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NUMERICAL ANALYSIS OF A MODEL FOR FERROMAGNETIC SHAPE MEMORY THIN FILMS

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Abstract. We give a model for the deformation and magnetization of a single crystal ferromagnetic shape memory thin film under the influence of an applied magnetic field. The energy is nonconvex since it models multiple phases and symmetry-related variants of the crystal structure. Nonconvexity is also presented by the magnetic saturation condition which requires the magnetization to have a constant magnitude.

We propose a class of finite element methods and prove a rate of convergence for the minimum thin film energy. In addition to the challenge of analyzing a nonconvex energy, the analysis overcomes the challenge presented by contributions to the energy that are naturally in the reference configuration for the elastic energy and in the spatial frame for the magnetic energy. We present numerical computations for the deformation and magnetization of a Ni_2MnGa thin film that exhibit the convergence rate given by analysis.

1. Introduction

Magnetostriction is the deformation of a solid in response to an applied magnetic field. If a martensitic material is also ferromagnetic, it is possible by applying a magnetic field to either induce the martensitic transformation (transition) or rearrange the variants of martensite . The resulting change of shape is reversible and is referred to the ferromagnetic shape memory effect [14].

Ferromagnetic shape memory crystals have been grown that exhibit a reversible shape change in response to an applied magnetic field [14], and the utilization of materials with this property in sensors, actuators, and micromachines are under rapid development. Single crystal ferromagnetic shape memory thin films have recently been grown [10] that have significant advantages over polycrystalline films [4].

We present a thin film model for ferromagnetic shape memory crystals that combines a rigorously derived thin film model for martensitic crystals [4, 7] with a rigorously derived thin film model for ferromagnetic crystals [11]. Our thin film energy is nonconvex since it must model the multiple phases and variants of the crystal structure. The space of admissible magnetizations is

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also nonconvex since the magnetic saturation condition requires the magnetization to have constant magnitude. We present numerical experiments in which the thin film model is applied to a Ni_2MnGa ferromagnetic shape memory crystal that undergoes a cubic to tetragonal structural phase transformation and is also ferromagnetic at temperatures below its structural martensitic transformation temperature [10].

We propose a class of finite element methods to approximate the thin film energy, and we prove that the energy converges with the rate that is observed in numerical experiments. We present the results of numerical experiments to compute the deformation and magnetization of a Ni_2MnGa thin film that exhibit the convergence rate that we have proven in Theorem 7.1.

Our analysis allows the film to have regions in which the film is in distinct energy wells of the energy density (variants of the crystal structure), and the numerical experiments approximate a thin film with this structure. The analysis must overcome the challenge presented by a free energy that includes elastic contributions defined in the reference configuration and magnetic contributions defined in the spatial frame, as well by the nonconvexity of the energy density.

In Section 2, we give a strain gradient model for ferromagnetic shape memory crystals, and in Section 3 we present a thin film model for the strain gradient energy. In Section 4, we present a sharp interface model for ferromagnetic shape memory crystals, and in Section 5 we present a thin film model for the sharp interface energy. We give a finite element approximation of the sharp interface thin film model in Section 6, and we give an analysis of the convergence of a class of finite element methods for the thin film energy in Section 7. Finally, in Section 8, we present the results of numerical experiments for a Ni_2MnGa film that show the convergence rate proven in Theorem 7.1.

2. The Strain Gradient Model for Ferromagnetic Shape Memory Crystals

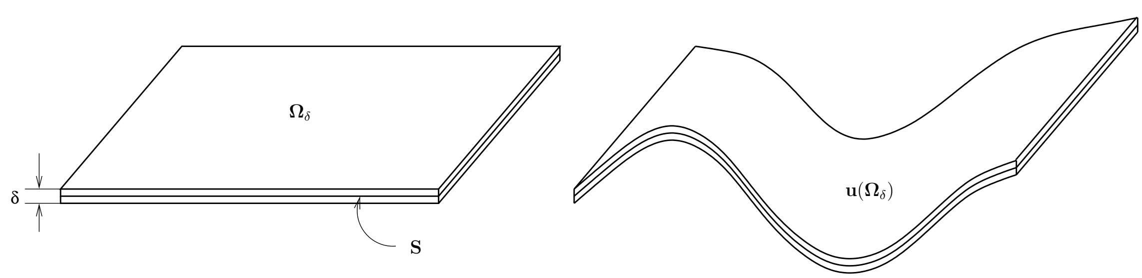


Figure 1. Reference and deformed configuration.

We consider a ferromagnetic shape memory thin film which in an undeformed state occupies the domain

$$\Omega_\delta = S \times \left(-\frac{\delta}{2}, \frac{\delta}{2}\right),$$

where $S \subset \mathbb{R}^2$ is a polygonal domain and $\delta \ll 1$ is the film thickness. Our model is based on the extension of geometrically nonlinear elasticity [8] to martensitic crystals [2]. We denote a deformation [8] of the film by $u(x) : \Omega_\delta \to \mathbb{R}^3$ (the deformation $u(x)$ is related to the displacement by $u(x) = x + v(x)$) , the domain of the deformed film by $u(\Omega_\delta)$, the magnetization of the film by $m(z) : u(\Omega_\delta) \to \mathbb{R}^3$. and the applied magnetic field by $h(z) : \mathbb{R}^3 \to \mathbb{R}^3$. We note that the deformation $u(x) : \Omega_\delta \to \mathbb{R}^3$ is naturally defined in material coordinates and the magnetization $m(z) : u(\Omega_\delta) \to \mathbb{R}^3$ is naturally defined in spatial coordinates. In the following, we will usually suppress the explicit dependence on the temperature θ since it will be considered to be constant in the crystal domain, Ω_δ.

The free energy of such a film can be given by [4, 5, 13]

$$\begin{aligned} \bar{e}^{(\delta)}(u,m) &= \int_{\Omega_\delta} \left\{ \kappa |D^2 u(x)|^2 + \varphi(\nabla u(x), m(u(x)), \theta) \right\} dx \\ &\quad + \int_{u(\Omega_\delta)} \left\{ \mu |\nabla_z m(z)|^2 - m(z) \cdot h(z) \right\} dz + e^{(\delta)}_{mag}(u,m) \\ &= \int_{\Omega_\delta} \left\{ \kappa |D^2 u(x)|^2 + \varphi(\nabla u(x), m(u(x)), \theta) \right\} dx \\ &\quad + \int_{\Omega_\delta} \left\{ \mu |\nabla_z m(u(x))|^2 \; - m(u(x)) \cdot h(u(x)) \right\} \det \nabla u(x) \, dx + e^{(\delta)}_{mag}(u,m), \end{aligned} \tag{2.1}$$

where κ is the surface energy coefficient, φ models the coupled elastic and magnetic anisotropic free energy densities, μ is the exchange energy coefficient, and $e^{(\delta)}_{mag}(u,m)$ is the magnetostatic energy given by

$$e^{(\delta)}_{mag}(u,m) = \frac{1}{2} \int_{\mathbb{R}^3} |\nabla \zeta(z)|^2 \, dz$$

with the scalar potential $\zeta(z) : \mathbb{R}^3 \to \mathbb{R}$ defined by

$$\nabla \cdot (-\nabla \zeta + \chi_{u(\Omega_\delta)} m) = 0 \text{ in } \mathbb{R}^3 \qquad \text{(magnetostatic equation)},$$

where $\chi_{u(\Omega_\delta)}$ is the characteristic function on $u(\Omega_\delta)$, that is, $\chi_{u(\Omega_\delta)}(z) = 1$ if $z \in u(\Omega_\delta)$ and $\chi_{u(\Omega_\delta)}(z) = 0$ if $z \notin u(\Omega_\delta)$.

The deformation u is constrained to satisfy the boundary condition

$$u(x) = u_0(x) \quad \text{for } x \in \partial S \times \left(-\frac{\delta}{2}, \frac{\delta}{2} \right),$$

where ∂S denotes the boundary of S. The magnetization satisfies the magnetic saturation condition

$$|m(u(x))| \; \det \nabla u(x) = m_s(\theta) \quad \text{for} \quad x \in \Omega_\delta,$$

where $|m|$ denotes the Euclidean norm and where the saturation magnetization $m_s(\theta) > 0$. However, we will use the simpler condition

$$|m(u(x))| = m_s(\theta) \quad \text{for} \quad x \in \Omega_\delta$$

without significant loss of accuracy [13].

The terms in (2.1) represent, from left to right, the surface energy, the combined elastic and magnetic anisotropy energies, the exchange energy, the interaction energy due to the applied magnetic field, and the magnetostatic energy. The "strain gradient" surface energy term above is defined by

$$\kappa \int_{\Omega_\delta} |D^2 u(x)|^2 \, dx = \kappa \int_{\Omega_\delta} \left[\sum_{i,j=1}^{3} \left| \frac{\partial^2 u(x)}{\partial x_i \partial x_j} \right|^2 \right] dx. \tag{2.2}$$

The energy density $\varphi(F, m, \theta)$ is a continuous function defined for $F \in \mathbb{R}^{3\times 3}$ and for $m \in \mathbb{R}^3$ that satisfy the magnetic saturation condition, $|m| = m_s(\theta)$. More properly, $\varphi(F, m, \theta)$ need only be defined on the group of nonsingular matrices F with positive determinant, but we will not impose this condition in this paper [8]. The energy density $\varphi(F, m, \theta)$ satisfies the following symmetries:

- $\varphi(RF, Rm, \theta) = \varphi(F, m, \theta)$ for all $R \in SO(3)$ (frame indifference);
- $\varphi(FQ, m, \theta) = \varphi(F, m, \theta)$ for all $Q \in \mathcal{G}$ (crystallographic symmetry);
- φ is even in m.

Here, $SO(3)$ is the group of proper rotations, and $\mathcal{G}$ is the symmetry group of the austenitic (high temperature) phase with transformation temperature θ_T, which for Ni_2MnGa is the cubic group. For θ below θ_T, φ has the energy wells

$$SO(3)[U_1(\theta), \pm m_1(\theta)] \cup \ldots \cup SO(3)[U_n(\theta), \pm m_n(\theta)], \tag{2.3}$$

where the U_i's are symmetry related energy minimizing variants of the martensitic (low temperature) phase and the m_i's are the preferred directions of magnetization (the easy axes) satisfying by the frame indifference and crystallographic symmetry properties the condition

$$\{(U_1, \pm m_1), \ldots, (U_n, \pm m_n)\} = \{(QU_1Q^T, \pm Q m_1) : Q \in \mathcal{G}\}.$$

We will assume that the elastic and magnetic anisotropy energy density has the smoothness $\varphi \in C^2(\mathbb{R}^{3\times 3} \times \mathbb{R}^3)$ and satisfies the growth condition that for $0 < C_L < C_U$ and $p > 3$ (to ensure that $u \in W^{1,p}(\Omega_\delta; \mathbb{R}^3)$ implies that $\det \nabla u \in L^1(\Omega_\delta)$)

$$C_L(|F|^p - 1) \le \varphi(F, m) \le C_U(|F|^p + 1) \quad \text{for all } F \in \mathbb{R}^{3\times 3} \text{ and } m \in \mathbb{R}^3,\ |m| = m_s. \tag{2.4}$$

3. The Thin Film Strain Gradient Model

Our thin film model for ferromagnetic shape memory crystals combines the rigorously derived thin film model for martensitic crystals of [4, 7] with the rigorously derived thin film model for ferromagnetic crystals of [11]. Our model [16] is that local minima (stable equilibria) (u, m) of the bulk energy $\bar{e}^{(\delta)}(u, m)$ are deformations satisfying

$$u(x_1, x_2, x_3) = y(x_1, x_2) + b(x_1, x_2)x_3 + o(x_3^2) \quad \text{for} \quad (x_1, x_2) \in S \quad \text{and} \quad x_3 \in \left(-\frac{\delta}{2}, \frac{\delta}{2}\right)$$

and magnetizations satisfying

$$m(u(x_1,x_2,x_3)) = M(x_1,x_2) + o(x_3) \quad \text{for} \quad (x_1,x_2) \in S \quad \text{and} \quad x_3 \in \left(-\frac{\delta}{2},\frac{\delta}{2}\right),$$

where the deformations $y(x_1,x_2) : S \to \mathbb{R}^3$ and $b(x_1,x_2) : S \to \mathbb{R}^3$ and the magnetizations $M(x_1,x_2) : S \to \mathbb{R}^3$ are local minima (stable equilibria) of the energy density per unit thickness

$$\begin{aligned}\bar{\mathcal{E}}(y,b,M) = &\int_S \left\{\kappa\left(|D^2y|^2 + 2|\nabla b|^2\right) + \varphi\left((y_{,1}|y_{,2}|b), M\right)\right\} dx_1dx_2 \\ &+ \int_S \left\{\mu|\nabla_{y(S)}M|^2 - M\cdot(h\circ y) + \frac{1}{2}\left[M\cdot(n\circ y)\right]^2\right\} \det(y_{,1}|y_{,2}|b)\, dx_1dx_2.\end{aligned} \tag{3.1}$$

We denoted by $(y_{,1}|y_{,2}|b)$ in (3.1) the deformation gradient matrix constructed from the column vectors $y_{,1}, y_{,2}$, and b . We also denoted by $\nabla_{y(S)}M$ the projection of the gradient ∇M onto the tangent plane of the surface $y(S)$. We note that the magnetization energy $e^{(\delta)}_{mag}(u,m)$ has been modeled by $\int_S \frac{1}{2}\left[M\cdot(n\circ y)\right]^2 \det(y_{,1}|y_{,2}|b)\, dx_1dx_2$ where the component of the magnetization normal to the film surface is given by $\left[M\cdot(n\circ y)\right](x_1,x_2) = M(x_1,x_2)\cdot n[y(x_1,x_2)]$ with $n[y(x_1,x_2)]$ being the normal to the film surface $y(S)$ at $y(x_1,x_2)$. In what follows, we will denote $M(x_1,x_2)$ by $m(x_1,x_2)$ and $(y_{,1}|y_{,2})$ by ∇y.

If we set $\kappa = 0$ and $\mu = 0$ in (3.1), then we have the variational problem:

$$\min\{\bar{\mathcal{E}}(y,b,m) : (y,b,m) \in \bar{\mathcal{A}}_{y_0}\}, \tag{3.2}$$

where the energy functional is now

$$\bar{\mathcal{E}}(y,b,m) = \int_S \left\{\varphi((\nabla y|b),m) + \left(\frac{1}{2}\left[m\cdot(n\circ y)\right]^2 - m\cdot(h\circ y)\right)\det(\nabla y|b)\right\} dx, \tag{3.3}$$

and the space of admissible functions is (after normalizing the magnetic saturation to $m_s = 1$)

$$\begin{aligned}\bar{\mathcal{A}}_{y_0} = \Big\{&(y,b,m) \in W^{1,p}(S;\mathbb{R}^3) \times L^p(S;\mathbb{R}^3) \times L^\infty(S;\mathbb{R}^3) : \\ &y(x) = y_0(x) \text{ for } x \in \partial S,\ \ |m(x)| = 1 \text{ for } x \in S\Big\}.\end{aligned} \tag{3.4}$$

We note that we should not expect a general existence theorem for (3.3) if the surface energy and the exchange energy are set to zero ($\kappa = 0$ and $\mu = 0$) since the deformation gradient and the magnetization can then oscillate on an infinitesimal length scale [2, 13, 17, 20]. However, the designs for the application of ferromagnetic shape memory films often use boundary conditions for which a piecewise smooth deformation and magnetization can be expected [3, 14]. We will thus analyze the approximation of the thin film energy (3.3) under the assumption that there exists a piecewise smooth minimizer. The neglect of the surface energy and the exchange energy in (3.3) allows the use of a conforming continuous finite element for y and a conforming piecewise constant finite element for b and m.

4. The Sharp Interface Model for Ferromagnetic Shape Memory Crystals

Martensitic materials often exhibit a deformation with nearly piecewise constant deformation gradient, but the strain gradient surface energy (2.2) gives an infinite energy if the deformation gradient is discontinuous across an interface. Thus, it is natural to consider the following total variation model of surface energy (see [7]) which gives a finite energy for a piecewise constant deformation gradient:

$$\int_{\Omega_\delta} \kappa |D(\nabla u)|, \tag{4.1}$$

where the total variation of a matrix valued function $u \in L^1(\Omega_\delta; \mathbb{R}^{3\times 3})$ is defined as

$$\int_{\Omega_\delta} |Du| = \sup \left\{ \sum_{i,\,j,\,k=1,2,3} \int_{\Omega_\delta} u_{ij}(x)\ \psi_{ijk,k}(x)\,dx : \psi \in \mathcal{C}_0^\infty(\Omega_\delta; \mathbb{R}^{3\times3\times3}),\ |\psi(x)| \le 1 \text{ for all } x \in \Omega_\delta \right\}.$$

The free energy of the film with the total variation surface energy is given by

$$\begin{aligned} e^{(\delta)}(u,m) = &\int_{\Omega_\delta} \Big\{ \kappa |D(\nabla u)| + \varphi\left(\nabla u(x), m\left(u(x)\right)\right) \Big\}\, dx \\ &+ \int_{\Omega_\delta} \Big\{ \mu |\nabla_z m(u(x))|^2\ - m(u(x)) \cdot h(u(x)) \Big\} \det \nabla u(x)\, dx + e^{(\delta)}_{mag}(u,m). \end{aligned} \tag{4.2}$$

5. The Sharp Interface Thin Film Model

If we model the surface energy by (4.1) in the bulk model (4.2), then the surface energy in the thin film model should be given by (see [7])

$$\int_S \kappa |D(\nabla y | \sqrt{2} b)|, \tag{5.1}$$

where the total variation of a matrix valued function $v \in L^1(S; \mathbb{R}^{m\times p})$ is defined as

$$\int_S |Dv| = \sup \left\{ \sum_{\substack{i=1,\dots,m \\ j=1,\dots,p \\ k=1,2}} \int_S v_{ij}(x)\ \psi_{ijk,k}(x) : \psi \in \mathcal{C}_0^\infty(S; \mathbb{R}^{m\times p\times 2}),\ |\psi(x)| \le 1 \text{ for all } x \in S \right\}.$$

For the thin model using the total variation surface energy (5.1) and neglecting the exchange energy ($\mu = 0$), we thus consider the variational problem

$$\min\{\mathcal{E}(y,b,m) : (y,b,m) \in \mathcal{A}_{y_0}\}, \tag{5.2}$$

where the energy functional is

$$\mathcal{E}(y,b,m) = \int_S \kappa\, |D(\nabla y|\sqrt{2}b)| + \int_S \Big\{ \varphi((\nabla y|b), m) + \Big(\frac{1}{2}(m\cdot n)^2 - m\cdot h\Big)\ \det(\nabla y|b) \Big\}\, dx. \tag{5.3}$$

The set of admissible functions is

$$\mathcal{A}_{y_0} = \Big\{(y,b,m) \in W^{1,p}(S;\mathbb{R}^3) \times L^p(S;\mathbb{R}^3) \times L^\infty(S;\mathbb{R}^3) : \\ y(x) = y_0(x) \text{ for } x \in \partial S,\ |m(x)| = 1 \text{ for } x \in S,\ \nabla y \in \mathrm{BV}(S),\ b \in \mathrm{BV}(S)\Big\}$$

where the subspace $\mathrm{BV}(S)$ of $L^1(S)$ is defined as

$$\mathrm{BV}(S) = \left\{ v : v \in L^1(S),\ \int_S |Dv| < \infty \right\}.$$

We note that if we consider the sharp interface thin film model in the limit of zero surface energy ($\kappa = 0$), then we have that the sharp interface energy $\mathcal{E}(y,b,m)$ is equal to the thin film energy $\bar{\mathcal{E}}(y,b,m)$ given in (3.3), and we can extend the space of admissible deformations $\mathcal{A}_{y_0}$ to $\bar{\mathcal{A}}_{y_0}$ given by (3.4).

6. The finite element approximation of the sharp interface thin film model

We now consider the finite element approximation of the total variation surface energy model (5.2). Let τ be a triangulation of the domain S, let K denote a triangle in τ, and let e denote an inter-element edge. Given an internal edge e and two triangles $K_1, K_2 \in \tau$ sharing the edge e, we define the jump across the edge e of a function ψ by

$$[\![\, \psi \,]\!]_e = \psi_{e,K_1} - \psi_{e,K_2},$$

where ψ_{e,K_i} denotes the trace on e of $\psi|_{K_i}$ for $i = 1, 2$. We denote by $P_1(\tau)$ the space of continuous piecewise linear functions on S, $P_0(\tau)$ the space of piecewise constant functions on S, and

$$\begin{aligned} \tilde{P}_1 \quad &= P_1(\tau) \times P_1(\tau) \times P_1(\tau), \\ \tilde{P}_{1,y_0} &= \{\, y_\tau \in \tilde{P}_1 : y_\tau = y_0 \quad \text{for } x \in \partial S \}\ , \\ \tilde{P}_0 \quad &= P_0(\tau) \times P_0(\tau) \times P_0(\tau), \\ \tilde{P}_0^\star \quad &= \{\, m_\tau \in \tilde{P}_0 : |m_\tau| = 1 \text{ for } x \in S\,\}\ , \end{aligned}$$

and the space of finite element trial functions by

$$\mathcal{A}_{\tau,y_0} = \tilde{P}_{1,y_0} \times \tilde{P}_0 \times \tilde{P}_0^\star. \tag{6.1}$$

A finite element approximation for the minimum energy of the total variation thin film model (5.2) can then be obtained from

$$\min\{\mathcal{E}(y_\tau, b_\tau, m_\tau) : (y_\tau, b_\tau, m_\tau) \in \mathcal{A}_{\tau,y_0}\}, \tag{6.2}$$

where the energy evaluated on the finite element functions in $\mathcal{A}_{\tau,y_0}$ takes the form

$$\begin{aligned}\mathcal{E}(y_\tau, b_\tau, m_\tau) = \kappa \sum_e \Big| [\![\nabla y_\tau | \sqrt{2} b_\tau]\!]_e \Big| \cdot |e| + \sum_{K\in\tau} \Big\{ \varphi((\nabla y_\tau | b_\tau)|_K, m_\tau|_K) \\ + \left[\frac{1}{2} m^2_{\tau,n}|_K - m_\tau|_K \cdot h|_K \right] \det((\nabla y_\tau | b_\tau)|_K) \Big\} \cdot |K|.\end{aligned} \tag{6.3}$$

In the above equation for the energy, $|e|$ denotes that length of the edge e, $|K|$ denotes the area of the triangle K, and

$$|[\![\nabla y_\tau | \sqrt{2} b_\tau]\!]_e| = (|[\![\nabla y_\tau]\!]_e|^2 + 2|[\![b_\tau]\!]_e|^2)^{1/2}.$$

We note that $\mathcal{A}_{\tau,y_0}$ is a conforming approximation of $\mathcal{A}_{y_0}$, and $(\nabla y_\tau, b_\tau, m_\tau)$ is a piecewise constant function with respect to the mesh τ for $(y_\tau, b_\tau, m_\tau) \in \mathcal{A}_{\tau,y_0}$. Hence, (6.3) is the exact evaluation of (5.3) and no numerical quadrature is needed.

7. Analysis of the finite element approximation of the thin film energy

In this section, we analyze the finite element approximation of the thin film model (3.2). We will use $||\cdot||_{k,q}$ and $|\cdot|_{k,q}$ to denote the standard norm and semi-norm of the Sobolev spaces $W^{k,q}(S)$ [1].

We assume that a quasi-regular family of triangulations $\{\tau\}$ with mesh size $|\tau|$ is given and that $\bar{\mathcal{A}}_{\tau,y_0}$ is a subset of a finite dimensional subspace of $\bar{\mathcal{A}}_{y_0}$. We also assume that $\bar{\mathcal{A}}_{\tau,y_0}$ has the approximation property that for every $q > 2$ there exists a positive constant, C, with the property that for every

$$(y, b, m) \in \bar{\mathcal{A}}_{y_0} \cap W^{2,q}(S; \mathbb{R}^3) \times W^{1,q}(S; \mathbb{R}^3) \times H^1(S; \mathbb{R}^3) \tag{7.1}$$

there exists $(y_\tau, b_\tau, m_\tau) \in \bar{\mathcal{A}}_{\tau,y_0}$ such that

$$\begin{aligned} &||y - y_\tau||_1 \le C|\tau||y|_2, \\ &||y - y_\tau||_{1,\infty} \le C|\tau|^{1-2/q}|y|_{2,q}, \\ &||b - b_\tau||_0 \le C|\tau||b|_1, \\ &||b - b_\tau||_\infty \le C|\tau|^{1-2/q}|b|_{1,q}, \\ &||m - m_\tau||_0 \le C|\tau||m|_1. \end{aligned} \tag{7.2}$$

We note that the finite element space $\mathcal{A}_{\tau,y_0} = \tilde{P}_{1,y_0} \times \tilde{P}_0 \times \tilde{P}_0^\star$ given in (6.1) satisfies $\mathcal{A}_{\tau,y_0} \subset \bar{\mathcal{A}}_{y_0}$ and the approximation property (7.2). More generally, finite element spaces $\bar{\mathcal{A}}_{\tau,y_0}$ where the deformations y_τ are continuous, piecewise polynomial functions, the b_τ are piecewise polynomial functions, and the m_τ are piecewise constant functions such that $|m_\tau(x)| = 1$ for all $x \in S$ will satisfy $\bar{\mathcal{A}}_{\tau,y_0} \subset \bar{\mathcal{A}}_{y_0}$ and the approximation property (7.2).

Our finite element approximation of the variational problem (3.2) is

$$\min\{\bar{\mathcal{E}}(y_\tau, b_\tau, m_\tau) : (y_\tau, b_\tau, m_\tau) \in \bar{\mathcal{A}}_{\tau,y_0}\}, \tag{7.3}$$

where the thin film energy $\bar{\mathcal{E}}(y,b,m)$ is defined as in (3.3) to be

$$\bar{\mathcal{E}}(y,b,m) = \int_S \left\{ \varphi((\nabla y|b),m) + \left(\frac{1}{2}(m\cdot n)^2 - m\cdot h\right)\det(\nabla y|b)\right\} dx. \tag{7.4}$$

We now show that the finite element minimization problem (7.3) does have a solution.

Lemma 7.1. *There exists a solution $(y_\tau, b_\tau, m_\tau) \in \bar{\mathcal{A}}_{\tau,y_0}$ to the finite element minimization problem (7.3).*

Proof. We define a norm $\|\cdot\|_\infty$ on $\bar{\mathcal{A}}_{\tau,y_0}$ by

$$\|(y_\tau,b_\tau,m_\tau)\|_\infty = \max_{x\in S}\{|y_\tau(x)|+|b_\tau(x)|+|m_\tau(x)|\} \quad \text{for } (y_\tau,b_\tau,m_\tau)\in\bar{\mathcal{A}}_{\tau,y_0}.$$

The thin film energy (7.4) is clearly continuous with respect to the norm $\|\cdot\|_\infty$. We can prove that the finite dimensional minimization problem (7.3) has a solution if we can show that for every $M>0$, there exists a $R_M>0$ such that

$$\|(y_k,b_k,m_k)\|_\infty \ge R_M,\ (y_k,b_k,m_k)\in\bar{\mathcal{A}}_{\tau,y_0}, \quad \text{implies that} \quad \bar{\mathcal{E}}(y_k,b_k,m_k)\ge M. \tag{7.5}$$

Since $|m_k(x)|=1,\ x\in S$, for $(y_k,b_k,m_k)\in\bar{\mathcal{A}}_{\tau,y_0}$, we have that $\|(y_k,b_k,m_k)\|_\infty\to\infty$ as $k\to\infty$ implies that $\max|y_k(x)|\to\infty$ as $k\to\infty$ or $\max|b_k(x)|\to\infty$ as $k\to\infty$.

Since $y_k=y_0$ on ∂S, we have that there exists a constant $C>$ such that [1]

$$\max_{x\in S}|y_k(x)| \le C\left(\max_{x\in S}|\nabla y_k(x)| + \max_{x\in\partial S}|y_0(x)|\right),$$

and we can conclude that $\max|y_k(x)|\to\infty$ as $k\to\infty$ implies that $\max|\nabla y_k(x)|\to\infty$ as $k\to\infty$.

Now we have since $\bar{\mathcal{A}}_{\tau,y_0}$ is a subset of a finite-dimensional space that there exists a constant $C_1>0$, dependent on τ, such that

$$\max_{x\in S}|\nabla^2 y_\tau(x)| \le C_1\max_{x\in S}|\nabla y_\tau(x)| \quad \text{and} \quad \max_{x\in S}|\nabla b_\tau(x)|\le C_1\max_{x\in S} b_\tau(x)|$$

for all $(y_\tau,b_\tau,m_\tau)\in\bar{\mathcal{A}}_{\tau,y_0}$. We thus have that there exists a constant $C_2>0$, dependent on C_1 and the polygonal domain S, such that for every $(y_\tau,b_\tau,m_\tau)\in\bar{\mathcal{A}}_{\tau,y_0}$ there exists a measurable set $\omega\subset S$ such that $\operatorname{meas}\omega\ge C_2$ with the property that

$$\min_{x\in\omega}|\nabla y_\tau(x)|\ge\frac{1}{2}\max_{x\in S}|\nabla y_\tau(x)| \quad \text{and} \quad \min_{x\in\omega}|b_\tau(x)|\ge\frac{1}{2}\max_{x\in S}|b_\tau(x)|. \tag{7.6}$$

Hence, we see from the growth condition (2.4) for $p>3$, from the bound $|\det F|\le 6|F|^3$ for $F\in\mathbb{R}^3$, and from the result (7.6) that $\max|y_k(x)|\to\infty$ as $k\to\infty$ or $\max|b_k(x)|\to\infty$ as $k\to\infty$ implies that $\bar{\mathcal{E}}(y_k,b_k,m_k)\to\infty$. □

We now define the magnetostatic and applied magnetic field energy densities

$$\begin{aligned}\psi_1(F,m) &= \frac{1}{2}(m\cdot n(F))^2\det(F),\\ \psi_2(F,m) &= -h\cdot m\det(F),\end{aligned} \tag{7.7}$$

for $F \in \mathbb{R}^{3\times 3}$ and $m \in \mathbb{R}^3,\ |m| = 1$. The normal vector $n(F)$ is given by

$$n(F) = \frac{N(F)}{|N(F)|}$$

for $N(F) = F_1 \times F_2$, where F_i is the ith column of F, or more explicitly

$$\begin{aligned} N_1(F) &= F_{2,1}F_{3,2} - F_{2,2}F_{3,1}\,, \\ N_2(F) &= F_{3,1}F_{1,2} - F_{3,2}F_{1,1}\,, \\ N_3(F) &= F_{1,1}F_{2,2} - F_{1,2}F_{2,1}\,. \end{aligned}$$

The following lemma gives bounds on the derivatives of the functions $N(F)$, $\psi_1(F,m)$, and $\psi_2(F,m)$.

Lemma 7.2. *For $\nu > 0$, we have that there exists a positive constant C such that*

$$\begin{aligned} \left|\frac{\partial n_i(F)}{F_{j,k}}\right| &\le C|F| \quad \text{for} \quad 1 \le i,j,k \le 3, \\ \left|\frac{\partial^2 n_i(F)}{\partial F_{j,k} F_{j',k'}}\right| &\le C|F|^2 \quad \text{for} \quad 1 \le i,j,j',k,k' \le 3, \end{aligned} \tag{7.8}$$

for all $F \in \mathbb{R}^{3\times 3}$ such that $|N(F)| \ge \nu$. We also have that

$$\begin{aligned} \left|\frac{\partial \psi_1}{\partial F}(F,m)\right| + \left|\frac{\partial \psi_1}{\partial m}(F,m)\right| &\le C(|F|^4 + 1), \\ \left|\frac{\partial \psi_2}{\partial F}(F,m)\right| + \left|\frac{\partial \psi_2}{\partial m}(F,m)\right| &\le C(|F|^3 + 1), \end{aligned} \tag{7.9}$$

and

$$\begin{aligned} \left|\frac{\partial^2 \psi_1}{\partial F^2}(F,m)\right| + \left|\frac{\partial^2 \psi_1}{\partial F \partial m}(F,m)\right| + \left|\frac{\partial^2 \psi_1}{\partial m^2}(F,m)\right| &\le C(|F|^5 + 1), \\ \left|\frac{\partial^2 \psi_2}{\partial F^2}(F,m)\right| + \left|\frac{\partial^2 \psi_2}{\partial F \partial m}(F,m)\right| + \left|\frac{\partial^2 \psi_2}{\partial m^2}(F,m)\right| &\le C(|F|^2 + 1), \end{aligned} \tag{7.10}$$

for all $F \in \mathbb{R}^{3\times 3}$ such that $|N(F)| \ge \nu$ and $m \in \mathbb{R}^3,\ |m| = 1$.

Proof. The bounds (7.8) follow from the quadratic dependence of $N(F)$ on F and from the inequality $|N(F)| \ge \nu > 0$.

The bounds (7.9) and (7.10) then follow from the cubic dependence of $\det(F)$ on F and the bounds (7.8). □

Theorem 7.1. *We consider the approximation of the thin film energy (7.4) by the finite element space $\bar{\mathcal{A}}_{\tau,y_0}$ with approximation properties (7.2). We further assume that the energy density $\varphi(F,m)$ is twice differentiable and that there exists a constant $C > 0$ such that*

$$\left|\frac{\partial^2 \varphi}{\partial F^2}(F,m)\right| + \left|\frac{\partial^2 \varphi}{\partial F \partial m}(F,m)\right| + \left|\frac{\partial^2 \varphi}{\partial m^2}(F,m)\right| \le C(|F|^{p-2} + 1) \tag{7.11}$$

for all $F \in \mathbb{R}^{3\times 3}$ *and* $m \in \mathbb{R}^3$, $|m| = 1$. *We also assume that a minimizer* $(\bar{y}, \bar{b}, \bar{m}) \in \bar{\mathcal{A}}_{y_0}$ *of the thin film energy (3.3) exists and satisfies the regularity assumption*

$$(\bar{y}, \bar{b}, \bar{m}) \in W^{2,q}(S;\mathbb{R}^3) \times W^{1,q}(S;\mathbb{R}^3) \times W^{1,2}(S;\mathbb{R}^3) \tag{7.12}$$

for $q > 2$, *and that there exists* $\nu > 0$ *such that*

$$|\bar{y}_{,1}(x) \times \bar{y}_{,2}(x)| \geq \nu > 0 \qquad \text{for all } x \in S. \tag{7.13}$$

Then there exists a constant, $C > 0$, *which depends on* $(\bar{y}, \bar{b}, \bar{m})$, *but is independent of the triangulation* τ, *such that*

$$0 \leq \min_{(\tilde{y}_\tau, \tilde{b}_\tau, \tilde{m}_\tau) \in \bar{\mathcal{A}}_{\tau, y_0}} \bar{\mathcal{E}}(\tilde{y}_\tau, \tilde{b}_\tau, \tilde{m}_\tau) - \min_{(y,b,m) \in \bar{\mathcal{A}}_{y_0}} \bar{\mathcal{E}}(y, b, m) \leq C|\tau|^2 \tag{7.14}$$

where $|\tau|$ *denotes the maximal mesh size in the triangulation* τ.

Proof. We define the total energy density $\eta(F, m)$ by

$$\eta(F, m) = \varphi(F, m) + \psi_1(F, m) + \psi_2(F, m) \quad \text{ for all } F \in \mathbb{R}^{3\times 3},\ m \in \mathbb{R}^3,\ |m| = 1,$$

where the magnetostatic and applied magnetic field energy densities $\psi_1(F, m)$ and $\psi_2(F, m)$ are given by (7.7). We then have that

$$\bar{\mathcal{E}}(y, b, m) = \int_S \eta((\nabla y|b), m)\, dx. \tag{7.15}$$

The first inequality in (7.14) is trivial since $\bar{\mathcal{A}}_{\tau,y_0} \subset \bar{\mathcal{A}}_{y_0}$. To prove the second inequality, we assume that $(y_\tau, b_\tau, m_\tau) \in \bar{\mathcal{A}}_{\tau,y_0}$ approximates $(\bar{y}, \bar{b}, \bar{m})$ with property (7.2). We then have that

$$\min_{(\tilde{y}_\tau, \tilde{b}_\tau, \tilde{m}_\tau) \in \bar{\mathcal{A}}_{\tau, y_0}} \bar{\mathcal{E}}(\tilde{y}_\tau, \tilde{b}_\tau, \tilde{m}_\tau) - \min_{(y,b,m) \in \bar{\mathcal{A}}_{y_0}} \bar{\mathcal{E}}(y, b, m) \leq \bar{\mathcal{E}}(y_\tau, b_\tau, m_\tau) - \bar{\mathcal{E}}(\bar{y}, \bar{b}, \bar{m})$$

since $(\bar{y}, \bar{b}, \bar{m}) \in \bar{\mathcal{A}}_{y_0}$ is a minimizer and $(y_\tau, b_\tau, m_\tau) \in \bar{\mathcal{A}}_{\tau,y_0}$. Now our task is to estimate $\bar{\mathcal{E}}(y_\tau, b_\tau, m_\tau) - \bar{\mathcal{E}}(\bar{y}, \bar{b}, \bar{m})$. We will use the notation

$$\begin{aligned}
&\bar{U} = (\bar{y}|\bar{b}, \bar{m}), \quad U_\tau = (y_\tau|b_\tau, m_\tau),\\
&e_\tau^U = (e_\tau^y|e_\tau^b, e_\tau^m) = (y_\tau|b_\tau, m_\tau) - (\bar{y}|\bar{b}, \bar{m}),\\
&y(t) = (1-t)\bar{y} + t y_\tau \qquad \text{for all } t \in [0,1],\\
&b(t) = (1-t)\bar{b} + t b_\tau \qquad \text{for all } t \in [0,1],\\
&m(t) = (1-t)\bar{m} + t m_\tau \qquad \text{for all } t \in [0,1],\\
&U(t) = (y(t)|b(t), m(t)) \qquad \text{for all } t \in [0,1],
\end{aligned}$$

and we define the scalar-valued function

$$J(t) = \bar{\mathcal{E}}(U(t)) \qquad \text{for all } t \in [0,1].$$

Since $(\bar{y}, \bar{b}, \bar{m})$ minimizes $\bar{\mathcal{E}}$, we have that $J'(0) = 0$ and from Taylor's theorem

$$\bar{\mathcal{E}}(y_\tau, b_\tau, m_\tau) - \bar{\mathcal{E}}(\bar{y}, \bar{b}, \bar{m}) = J(1) - J(0) = -\int_0^1 J''(t)(t-1)\, dt. \tag{7.16}$$

We have that

$$J''(t) = \delta^2 \bar{\mathcal{E}}(U(t))(e_\tau^U, e_\tau^U),$$

where

$$\begin{aligned}
\delta^2 \bar{\mathcal{E}}(U(t))(e_\tau^U, e_\tau^U) &= \int_S \left\{ \frac{\partial^2 \eta}{\partial F^2}(\nabla y | b, m)(\nabla e_\tau^y | e_\tau^b, \nabla e_\tau^y | e_\tau^b) \right. \\
&\quad \left. + 2 \frac{\partial^2 \eta}{\partial F \partial m}(\nabla y | b, m)(\nabla e_\tau^y | e_\tau^b, e_\tau^m) + \frac{\partial^2 \eta}{\partial m^2}(\nabla y | b, m)(e_\tau^m, e_\tau^m) \right\} dx \\
&= \int_S \left\{ \frac{\partial^2 \varphi}{\partial F^2}(\nabla y | b, m)(\nabla e_\tau^y | e_\tau^b, \nabla e_\tau^y | e_\tau^b) + 2 \frac{\partial^2 \varphi}{\partial F \partial m}(\nabla y | b, m)(\nabla e_\tau^y | e_\tau^b, e_\tau^m) \right. \\
&\quad \left. + \frac{\partial^2 \varphi}{\partial m^2}(\nabla y | b, m)(e_\tau^m, e_\tau^m) \right\} dx \\
&\quad + \int_S \left\{ \frac{\partial^2 \psi_1}{\partial F^2}(\nabla y | b, m)(\nabla e_\tau^y | e_\tau^b, \nabla e_\tau^y | e_\tau^b) + 2 \frac{\partial^2 \psi_1}{\partial F \partial m}(\nabla y | b, m)(\nabla e_\tau^y | e_\tau^b, e_\tau^m) \right. \\
&\quad \left. + \frac{\partial^2 \psi_1}{\partial m^2}(\nabla y | b, m)(e_\tau^m, e_\tau^m) \right\} dx \\
&\quad + \int_S \left\{ \frac{\partial^2 \psi_2}{\partial F^2}(\nabla y | b, m)(\nabla e_\tau^y | e_\tau^b, \nabla e_\tau^y | e_\tau^b) + 2 \frac{\partial^2 \psi_2}{\partial F \partial m}(\nabla y | b, m)(\nabla e_\tau^y | e_\tau^b, e_\tau^m) \right. \\
&\quad \left. + \frac{\partial^2 \psi_2}{\partial m^2}(\nabla y | b, m)(e_\tau^m, e_\tau^m) \right\} dx.
\end{aligned} \tag{7.17}$$

Now it follows from (7.2) and (7.12) that there exists a positive constant C such that

$$\|\bar{y} - y_\tau\|_{1,\infty} \leq C|\tau|^{1-2/q}, \tag{7.18}$$

and we can thus conclude from (7.13) that for $|\tau|$ sufficiently small

$$|y_{,1} \times y_{,2}| \geq \nu/2 > 0 \qquad \text{for all } x \in S,\ t \in [0,1].$$

We also have from (7.12) and (7.18) that there exists a constant $C > 0$ such that for $|\tau|$ sufficiently small

$$|\nabla y| + |b| \leq C \qquad \text{for all } x \in S,\ t \in [0,1]. \tag{7.19}$$

We can then conclude from (7.10), (7.11), and (7.17) that there exists $C > 0$ such that

$$\delta^2 \bar{\mathcal{E}}(U(t))(e_\tau^U, e_\tau^U) \leq C \left(\|\nabla e_\tau^y\|^2 + \|e_\tau^b\|^2 + \|e_\tau^m\|^2 \right) \qquad \text{for all } t \in [0,1].$$

The result (7.14) now follows from (7.2), (7.12), and (7.16). $\square$

If the energy density, $\varphi(F,m)$, is nonconvex, then we do not expect that the solution of the minimization problem (7.4) will satisfy the regularity

$$(\bar{y},\bar{b},\bar{m}) \in W^{2,q}(S;\mathbb{R}^3)\times W^{1,q}(S;\mathbb{R}^3)\times W^{1,2}(S;\mathbb{R}^3)$$

unless the solution represents only one phase or variant [2,17]. In the next section, we will study the numerical computation of a thin film with two variants, and we will observe the second order convergence of the energy as given in Theorem 7.1. This can be explained by noting that the approximation properties (7.2) hold if $(\bar{y},\bar{b},\bar{m})$ is smooth except across an interface that is on the boundaries of triangles in the finite element mesh, which is the case for the computation of the film studied in the next section and shown in Figure 5. In this case, the proof of Theorem 7.1 is easily extended to give second order convergence of the energy.

To attempt to prove a classical estimate for the error in the deformation gradient and magnetization, we let $(\bar{y}_\tau,\bar{b}_\tau,\bar{m}_\tau)\in\bar{\mathcal{A}}_{\tau,y_0}$ be a minimizer of

$$\min_{(\tilde{y}_\tau,\tilde{b}_\tau,\tilde{m}_\tau)\in\bar{\mathcal{A}}_{\tau,y_0}} \bar{\mathcal{E}}(\tilde{y}_\tau,\tilde{b}_\tau,\tilde{m}_\tau).$$

We now use the notation

$$\begin{aligned}
&\bar{U}=(\bar{y}|\bar{b},\bar{m}),\quad \bar{U}_\tau=(\bar{y}_\tau|\bar{b}_\tau,\bar{m}_\tau),\\
&\bar{e}^U_\tau=(\bar{e}^y_\tau|\bar{e}^b_\tau,\bar{e}^m_\tau)=(\bar{y}_\tau|\bar{b}_\tau,\bar{m}_\tau)-(\bar{y}|\bar{b},\bar{m}),\\
&y(t)=(1-t)\bar{y}+t\bar{y}_\tau \qquad \text{for all } t\in[0,1],\\
&b(t)=(1-t)\bar{b}+t\bar{b}_\tau \qquad \text{for all } t\in[0,1],\\
&m(t)=(1-t)\bar{m}+t\bar{m}_\tau \qquad \text{for all } t\in[0,1],\\
&U(t)=(y(t)|b(t),m(t)) \qquad \text{for all } t\in[0,1].
\end{aligned}$$

Since $(\bar{y},\bar{b},\bar{m})$ minimizes $\bar{\mathcal{E}}$, we have again from Taylor's theorem that

$$\bar{\mathcal{E}}(\bar{y}_\tau,\bar{b}_\tau,\bar{m}_\tau)-\bar{\mathcal{E}}(\bar{y},\bar{b},\bar{m})=\int_0^1\delta^2\bar{\mathcal{E}}(U(t))(\bar{e}^U_\tau,\bar{e}^U_\tau)(1-t)\,dt, \tag{7.20}$$

where now

$$\begin{aligned}
\delta^2\bar{\mathcal{E}}(U(t))(\bar{e}^U_\tau,\bar{e}^U_\tau)=\int_S\Big\{&\frac{\partial^2\eta}{\partial F^2}(\nabla y|b,m)(\nabla\bar{e}^y_\tau|\bar{e}^b_\tau,\nabla\bar{e}^y_\tau|\bar{e}^b_\tau)\\
&+2\frac{\partial^2\eta}{\partial F\partial m}(\nabla y|b,m)(\nabla\bar{e}^y_\tau|\bar{e}^b_\tau,\bar{e}^m_\tau)+\frac{\partial^2\eta}{\partial m^2}(\nabla y|b,m)(\bar{e}^m_\tau,\bar{e}^m_\tau)\Big\}\,dx.
\end{aligned} \tag{7.21}$$

If an estimate such as (7.14) holds, then we have that

$$0\le\bar{\mathcal{E}}(\bar{y}_\tau,\bar{b}_\tau,\bar{m}_\tau)-\bar{\mathcal{E}}(\bar{y},\bar{b},\bar{m})=\int_0^1\delta^2\bar{\mathcal{E}}(U(t))(\bar{e}^U_\tau,\bar{e}^U_\tau)(1-t)\,dt\le C|\tau|^2.$$

Hence, we see that we can prove an estimate for $\bar{e}^U_\tau = \left(\bar{e}^y_\tau | \bar{e}^b_\tau, \bar{e}^m_\tau\right)$ if there exists a positive constant C such that

$$\delta^2 \bar{\mathcal{E}}(U(t))(\bar{e}^U_\tau, \bar{e}^U_\tau) \geq C \int_S \left(|\nabla \bar{e}^y_\tau|^2 + |\bar{e}^b_\tau|^2 + |\bar{e}^m_\tau|^2 \right) dx \tag{7.22}$$

for all $t \in [0,1]$. The coercivity condition (7.22) will follow if there exists a positive constant C such that we have the convexity condition

$$\begin{aligned} &\frac{\partial^2 \eta}{\partial F^2}(\nabla y|b,m)(\nabla \bar{e}^y_\tau|\bar{e}^b_\tau, \nabla \bar{e}^y_\tau|\bar{e}^b_\tau) + 2\frac{\partial^2 \eta}{\partial F \partial m}(\nabla y|b,m)(\nabla \bar{e}^y_\tau|\bar{e}^b_\tau, \bar{e}^m_\tau) + \frac{\partial^2 \eta}{\partial m^2}(\nabla y|b,m)(\bar{e}^m_\tau, \bar{e}^m_\tau) \\ &\qquad \geq C \left(|\nabla \bar{e}^y_\tau|^2 + |\bar{e}^b_\tau|^2 + |\bar{e}^m_\tau|^2 \right) \end{aligned} \tag{7.23}$$

for all $t \in [0,1]$ and all $x \in S$. Such a convexity condition (7.23) cannot be expected if $\left((\nabla \bar{y}|\bar{b}), \bar{m}\right)$ and $\left((\nabla \bar{y}_\tau|\bar{b}_\tau), \bar{m}_\tau\right)$ do not both take values in the same energy well of $\eta(F,m)$ for all $x \in S$. We recall that the energy wells are not strictly convex because of the rotational invariance (2.3), so the convexity condition (7.23) may fail even if both $\left((\nabla \bar{y}|\bar{b}), \bar{m}\right)$ and $\left((\nabla \bar{y}_\tau|\bar{b}_\tau), \bar{m}_\tau\right)$ take values in the same energy well of $\eta(F,m)$ for all $x \in S$. A possible program to analyze the convergence of $(\bar{y}_\tau, \bar{b}_\tau, \bar{m}_\tau)$ would be to attempt to extend the analysis of Theorem 7.1 to solutions with microstructure such as obtained in [15, 17–20].

8. Numerical Computation of a Thin Film with Two Variants

In this section, we present numerical results for the finite element approximation of the thin film model (7.4) at a fixed temperature below the transformation temperature. We consider the ferromagnetic shape memory material Ni_2MnGa which undergoes a cubic to tetragonal phase transformation. We construct a frame indifferent free energy density with minima at the wells

$$SO(3)[U_1, \pm m_1] \cup SO(3)[U_2, \pm m_2] \cup SO(3)[U_3, \pm m_3],$$

where the three martensitic variants are given by

$$U_1 = \begin{pmatrix} \beta & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \alpha \end{pmatrix}, \qquad m_1 = m_s(1,0,0)^T,$$

$$U_2 = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \beta & 0 \\ 0 & 0 & \alpha \end{pmatrix}, \qquad m_2 = m_s(0,1,0)^T,$$

$$U_3 = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \beta \end{pmatrix}, \qquad m_3 = m_s(0,0,1)^T.$$

The transformation strains $\alpha = 1.0163$ and $\beta = 0.9555$ are ratios of lattice parameters of the martensitic and austenitic phase.

We note that if at some point x the deformation gradient is on one of the energy wells, namely,

$$(\nabla \bar{y}|\bar{b})(x) = RU_1 = R\begin{pmatrix}\beta & 0 & 0\\ 0 & \alpha & 0\\ 0 & 0 & \alpha\end{pmatrix},$$

then

$$\bar{y}_{,1} \times \bar{y}_{,2} = R\begin{pmatrix}\beta\\ 0\\ 0\end{pmatrix} \times R\begin{pmatrix}0\\ \alpha\\ 0\end{pmatrix} = \operatorname{cof} R\begin{pmatrix}\beta\\ 0\\ 0\end{pmatrix} \times \begin{pmatrix}0\\ \alpha\\ 0\end{pmatrix}.$$

Thus,

$$|\bar{y}_{,1} \times \bar{y}_{,2}| = \alpha\beta > 0,$$

and if the deformation gradient $(\nabla \bar{y}|\bar{b})(x)$ of the minimizer is not far away from the energy wells, the assumption

$$|\bar{y}_{,1} \times \bar{y}_{,2}| \geq \nu > 0 \quad \text{for all } x \in S$$

is justified.

For our computations with the thin film energy (7.4), we use the frame-indifferent energy density

$$\varphi(F, m) = \varphi_1(F) + \varphi_2(F, m) \quad \text{for all } F \in \mathbb{R}^{3\times 3},\ m \in \mathbb{R}^3,\ |m| = m_s,$$

with the elastic energy density given by

$$\begin{aligned}\varphi_1(F) = c_1(\det F - \alpha^2\beta)^2 + c_2(C_{12}^2 + C_{13}^2 + C_{23}^2)\\ + c_3\left((\operatorname{tr}C - (2\alpha^2 + \beta^2))^2 + (C_{11}C_{22}C_{33} - \alpha^4\beta^2)^2\right) \quad \text{for all } F \in \mathbb{R}^{3\times 3},\end{aligned}$$

where c_1, c_2 and c_3 are positive elastic moduli and $C = F^T F$ is the right Cauchy-Green strain. The magnetic anisotropic free energy density is given by

$$\varphi_2(F, m) = \frac{\kappa_u}{\alpha^2 - \beta^2}\left|\frac{m \cdot Bm}{m \cdot m} - \beta^2\right| \quad \text{for all } F \in \mathbb{R}^{3\times 3},\ m \in \mathbb{R}^3,\ |m| = m_s,$$

where $B = FF^T$ is the left Cauchy-Green strain and $\kappa_u > 0$ is the magnetic anisotropy constant of the material. We used the non-physical dimensionless elastic moduli $c_1 = c_2 = c_3 = 30$, magnetic anisotropic constant $\kappa_u = 40$, saturation magnetization $m_s = 1$, and applied magnetic field $h = (0, 0, 1)$.

We take as our computational domain S the unit square $(0,1)\times(0,1)$, and we use the regular cross diagonal triangular mesh shown in Figure 6(a). We construct a finite element space $\bar{\mathcal{A}}_{\tau,y_0} \subset \bar{\mathcal{A}}_{y_0}$ satisfying (7.2) by approximating the deformation y by the reduced HCT (Hsieh-Clough-Tocher) element, $\mathcal{P}_{HCT}(\tau)$ [9]. We then construct $\bar{\mathcal{A}}_{\tau,y_0} \subset \bar{\mathcal{A}}_{y_0}$ by

$$\begin{aligned}\tilde{\mathcal{P}}_{HCT} &= \mathcal{P}_{HCT}(\tau) \times \mathcal{P}_{HCT}(\tau) \times \mathcal{P}_{HCT}(\tau),\\ \tilde{\mathcal{P}}_{HCT,y_0} &= \{\, y \in \tilde{\mathcal{P}}_{HCT} : y = y_0 \quad \text{for } x \in \partial S\},\end{aligned}$$

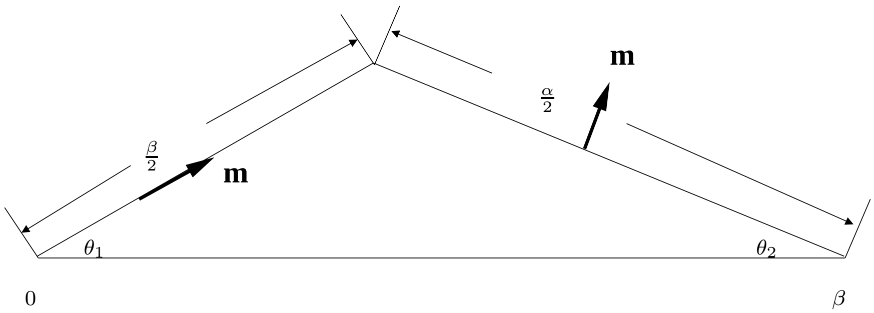


FIGURE 2. Schematic picture of the initial state at a cross section with fixed x_2.

$$\bar{\mathcal{A}}_{\tau,y_0} \quad = \tilde{\mathcal{P}}_{HCT,y_0} \times \tilde{P}_1 \times \tilde{P}_0^{\star},$$

where $\tilde{P}_1$ and $\tilde{P}_0^{\star}$ are defined in Section 6. We note that the finite element space is also a subspace of the admissible functions for the strain gradient energy (3.1) when $\kappa > 0$ and $\mu = 0$.

We only constrain y to satisfy the Dirichlet boundary condition on $\Gamma_D = \{x_1 = 0\} \cup \{x_1 = 1\}$, not the entire ∂S. Since Γ_D has a positive 1-dimensional measure, the analysis we did in the previous sections still holds. For a given mesh, we use N to denote the number of edges along each side of S, thus N is inversely proportional to the mesh size and $N = 16$ in Figure 6(a). In our computation of $\bar{\mathcal{E}}(y, b, m)$, we used the 12 point Gaussian quadrature rule [12, page 173].

We obtain the initial state by first deforming the left half of the reference state to the first variant with deformation gradient U_1 and magnetization m_1, and the right half of the reference state to the third variant with deformation gradient U_3 and magnetization m_3, and by then bending the film along the center $x_1 = 1/2$ to apply a rotation of angle $\theta_1 = \arccos(\frac{5}{4} - \frac{\alpha^2}{4\beta^2})$ for $0 < x_1 < 1/2$ and a rotation of angle $-\theta_2 = -\arccos(\frac{3\beta}{4\alpha} + \frac{\alpha}{4\beta})$ for $1/2 < x_1 < 1$, (see Figure 2 for the schematic picture).

The equations for the initial data are given by

$$y_1(x) = \beta x_1 \cdot \cos\theta_1, \qquad y_2(x) = \alpha x_2, \qquad y_3(x) = \beta x_1 \cdot \sin\theta_1,$$
$$b_1(x) = -\alpha \sin\theta_1, \qquad b_2(x) = 0, \qquad b_3(x) = \alpha\cos\theta_1,$$
$$m_1(x) = \cos\theta_1, \qquad m_2(x) = 0, \qquad m_3(x) = \sin\theta_1,$$

for $0 \le x_1 \le \frac{1}{2}$, and

$$y_1(x) = \beta - \alpha(1 - x_1)\cos\theta_2, \qquad y_2(x) = \alpha x_2, \qquad y_3(x) = \alpha(1 - x_1)\sin\theta_2,$$
$$b_1(x) = \beta \sin\theta_2, \qquad b_2(x) = 0, \qquad b_3(x) = \beta\cos\theta_2,$$
$$m_1(x) = \sin\theta_2, \qquad m_2(x) = 0, \qquad m_3(x) = \cos\theta_2,$$

for $\frac{1}{2} \le x_1 \le 1$.

We start with a coarse mesh $N = 8$ and the roof-shaped initial state for (y, b, m) on this mesh as shown in Figure 3(a). In this figure, the green arrow in the upper right corner indicates the direction of the applied magnetic field. In the deformed configuration of the film, we distinguish different martensitic variants by coloring each triangle according to the energy well closest to the deformation gradient in that triangle [17]. More precisely, we assign the martensitic variant i to a given triangle K with right Cauchy-Green strain $C = F^T F$ for $F = (\nabla y|b)$ if and only if

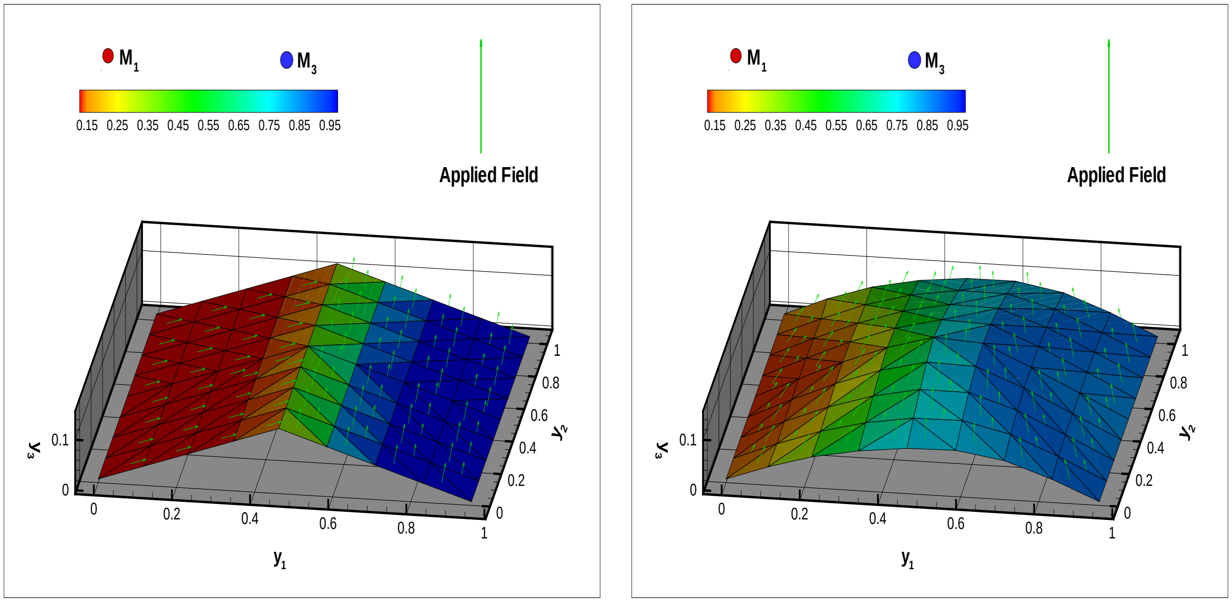
$$|C - C_i|_K = \min\{|C - C_1|_K, |C - C_3|_K\},$$

where $C_i = U_i^T U_i$, for $i = 1$ or 3, and $|\cdot|$ is the Euclidean norm of the matrix. Since we used the reduced HCT element for the deformation y and the continuous, piecewise linear element for b, on each triangle the deformation gradient F is calculated by averaging its value at the 3 vertices of the triangle. We represent the variant U_1 by red and U_3 by blue. In each deformed triangle, we represent the magnetization m by plotting a green arrow starting from the barycenter of the triangle with constant length and in the direction of of m. Here no averaging is needed since the piecewise constant element is used for m.

We used the Polak-Ribière nonlinear conjugate gradient (NCG) method to minimize the energy in the finite element space $\bar{\mathcal{A}}_{\tau,y_0}$ with the above deformation and magnetization as the initial state [6]. The NCG method converged to the local minimizer of the energy shown in Figure 3(b). We then obtained local minimizers on increasingly finer meshes by refining the mesh by increasing N successively by 8, interpolating the local minimizer (y, b, m) at the coarser mesh to the finer mesh, and minimizing the energy. Figure 4 gives the result for $N = 16$, with (a) being the interpolant of the minimizer at $N = 8$ and (b) being the minimizer at $N = 16$. We observe that the energy minimizing deformation is stable upon mesh refinement and consists of two regions, one with right Cauchy-Green strain near U_1^2 and one with right Cauchy-Green strain near U_3^2.

Figure 6(b) is a plot of the energy versus mesh size, and it indicates that the energy error decays as a certain power of the mesh size. We determine the order of convergence of the energy by assuming that the error $E(N)$ as a function of N is asymptotically of the form $E(N) = b/N^\gamma$, where γ is the order and b is a constant. If the minimum energy value attained in the continuous function space is a, then the minimum energy value attained in the discrete function space with mesh size N is asymptotically $\mathcal{E}(N) = a + E(N) = a + b/N^\gamma$. Since there are 3 parameters a, b, γ in the equation $\mathcal{E}(N) = a + b/N^\gamma$, for 3 distinct pairs of values $(N_i, \mathcal{E}_i)$, $(N_j, \mathcal{E}_j)$, and $(N_k, \mathcal{E}_k)$, we can eliminate b and γ to obtain a as the root of the equation

$$F(a; N_i, N_j, N_k, \mathcal{E}_i, \mathcal{E}_j, \mathcal{E}_k) = \frac{\mathcal{E}_j + \mathcal{E}_k - 2a}{\frac{\mathcal{E}_j - a}{\mathcal{E}_i - a} + \left(\frac{N_i}{N_k}\right)^{\log\left(\frac{\mathcal{E}_k - a}{\mathcal{E}_j - a}\right)/\log\left(\frac{N_j}{N_k}\right)}} + a - \mathcal{E}_i = 0. \tag{8.1}$$



(a) (b)

FIGURE 3. Initial value and minimizer for $N = 8$.

We plot in Figure 7(a) the graph of $y = F(a; N_i, N_j, N_k, \mathcal{E}_i, \mathcal{E}_j, \mathcal{E}_k)$ for $(N_7, \mathcal{E}_7)$, $(N_9, \mathcal{E}_9)$, $(N_{11}, \mathcal{E}_{11})$ and for $(N_8, \mathcal{E}_8)$, $(N_{10}, \mathcal{E}_{10})$, $(N_{12}, \mathcal{E}_{12})$ to give two approximations to the root of (8.1) as the intersection of the graph with the horizontal axis $y = 0$. We then averaged the two roots to obtain $a = -0.6074$.

Having obtained a, we can approximate the energy error as $E(N) = \mathcal{E}(N) - a = b/N^{\gamma}$ and obtain the order of convergence of the energy as the slope of $\log E(N)$ as a function of $\log N$. For two consecutive points (N_i, E_i) and (N_{i+1}, E_{i+1}), we calculate the approximate convergence order between these two points as $\gamma_i = -(\log E_{i+1} - \log E_i)/(\log N_{i+1} - \log N_i)$. Figure 7(b) is the plot of γ_i versus $(N_i + N_{i+1})/2$, and we observe a convergence rate that is close to the second order convergence as predicted by Theorem 7.1.

In summary, we have proposed a model for a single crystal ferromagnetic shape memory thin film and presented a finite element numerical approximation of the model. We have given an error analysis of our finite element approximation and numerical results that exhibit the order of convergence that we have obtained in Theorem 7.1.

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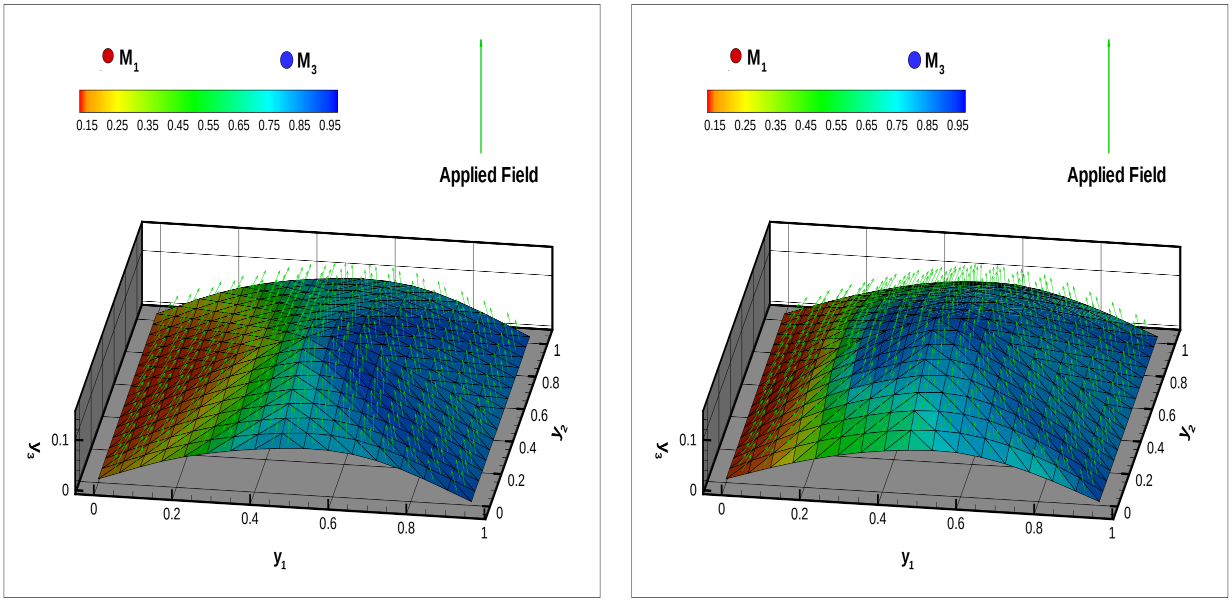
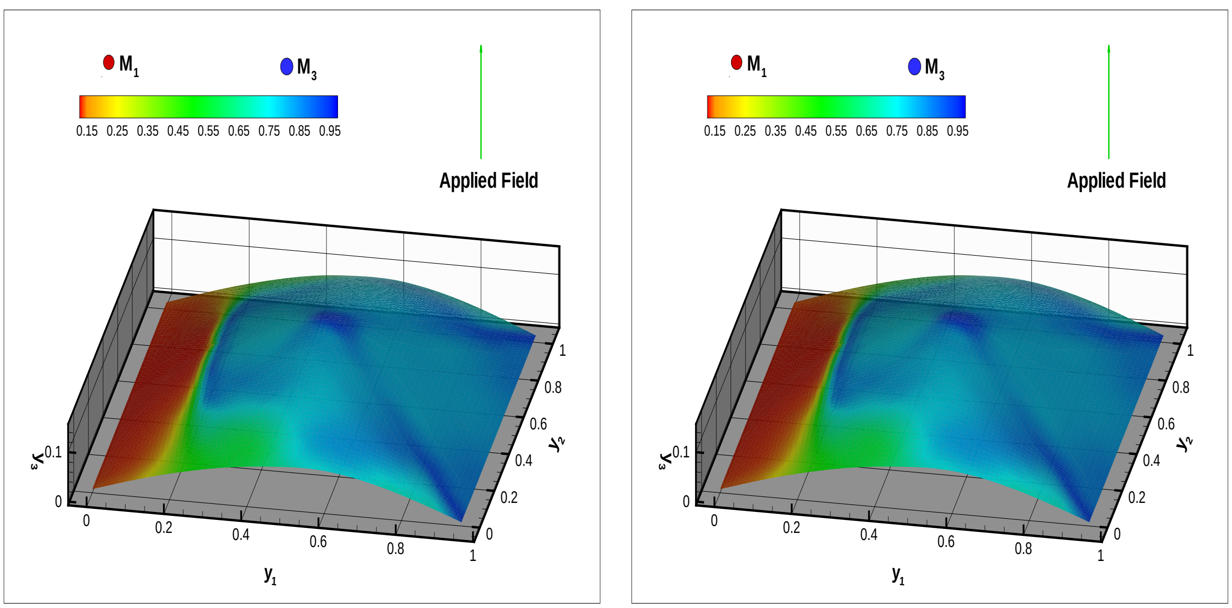


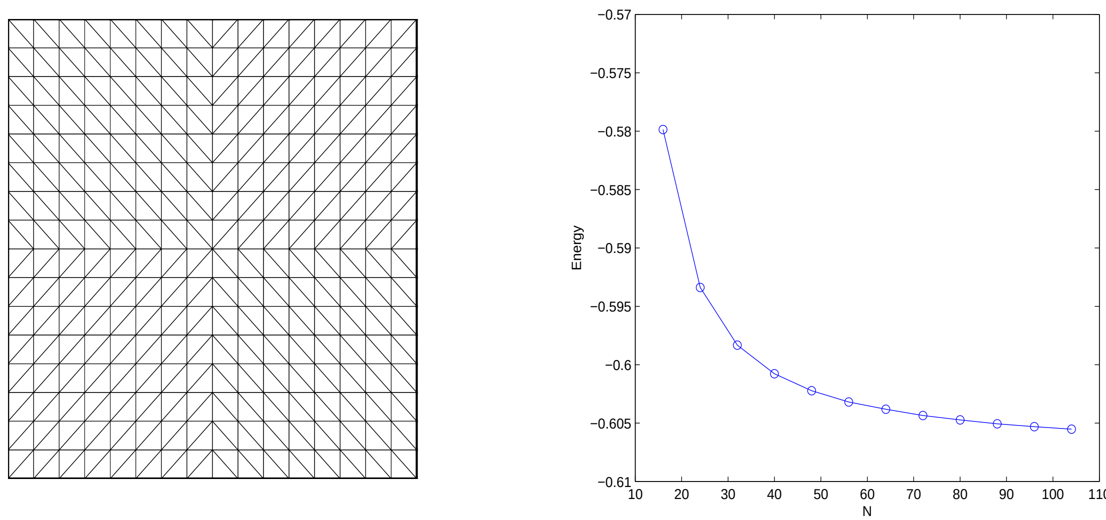
(a) (b)

FIGURE 4. Initial value and minimizer for $N = 16$.



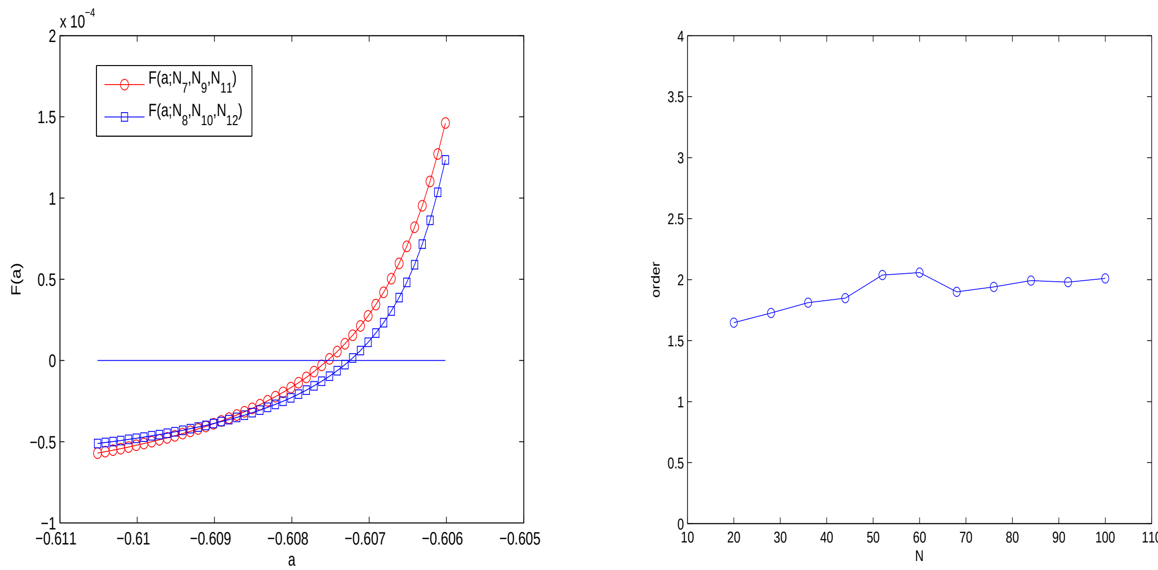
(a) (b)

FIGURE 5. Initial value and minimizer for $N = 80$.



(a) (b)

FIGURE 6. Triangular mesh and energy versus mesh size.



(a) (b)

FIGURE 7. Convergence order of the energy.

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