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Computational modeling of microstructure

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Abstract

Many materials such as martensitic or ferromagnetic crystals are observed to be in metastable states exhibiting a fine-scale, structured spatial oscillation called microstructure; and hysteresis is observed as the temperature, boundary forces, or external magnetic field changes. We have developed a numerical analysis of microstructure and used this theory to construct numerical methods that have been used to compute approximations to the deformation of crystals with microstructure.

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1. Introduction

Martensitic crystals are observed to be in metastable states that can be modeled by local minima of the energy [1, 2, 11, 17, 19, 25, 33, 36]

$$\mathcal{E}(y) = \int_\Omega \phi(\nabla y(x), \theta(x))\, dx + \text{interfacial energy} + \text{loading energy} \tag{1.1}$$

where $\Omega \subset \mathbb{R}^3$ is the reference configuration of the crystal, $y(x) : \Omega \to \mathbb{R}^3$ is the deformation that may be constrained on the boundary $\partial\Omega$, and $\theta(x) : \Omega \to \mathbb{R}$ is the temperature. The frame-indifferent elastic energy density $\phi(F, \theta) : \mathbb{R}^{3\times 3} \times \mathbb{R} \to \mathbb{R}$ is minimized at high temperature $\theta \geq \theta_T$ on SO(3) and at low temperature $\theta \leq \theta_T$

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on the martensitic variants $\mathcal{U} = \mathrm{SO}(3)U_1 \cup \cdots \cup \mathrm{SO}(3)U_N$ where the $U_i \in \mathbb{R}^{3\times 3}$ are symmetry-related transformation strains satisfying

$$\{\, R_i^T U_1 R_i : R_i \in \mathcal{G} \,\} = \{\, U_1, \ldots, U_N \,\}$$

for the symmetry group $\mathcal{G}$ of the high temperature (austenitic) phase. The loading energy above results from applied boundary forces.

Microstructure occurs when the deformation gradient oscillates in space among the $\mathrm{SO}(3)U_i$ to enable the deformation to attain a lower energy than could be attained by a more homogeneous state [1, 25]. The simplest microstructure is a laminate in which the deformation gradient oscillates between $R_iU_i \in \mathrm{SO}(3)U_i$ and $R_jU_j \in \mathrm{SO}(3)U_j$ for $i \neq j$ in parallel layers of fine scale, but more complex microstructure is observed in nature and is predicted by the theory [2, 25].

We have developed numerical methods for the computation of microstructure in martensitic and ferromagnetic crystals and validated these methods by the development of a numerical analysis of microstructure [4, 6, 12, 14, 16, 22, 25–28]. Related results are given in [9, 10, 15, 21, 24, 31, 32, 34]. For martensitic crystals, we have given error estimates for stable quantities such as nonlinear integrals $\int_\Omega f(x, \nabla y(x))\, dx$ for smooth functions $f(x, F) : \Omega \times \mathbb{R}^{3\times 3} \to \mathbb{R}$ and for the local volume fractions (Young measure) of the variants $\mathrm{SO}(3)U_i$ even though pointwise values of the deformation gradient are not stable under mesh refinement.

To model the evolution of metastable states, we have developed a computational model that nucleates the first order phase change since otherwise the crystal would remain stuck in local minima of the energy as the temperature or boundary forces are varied [8]. Our finite element model for the quasi-static evolution of the martensitic phase transformation in a thin film nucleates regions of the high temperature phase during heating and regions of the low temperature phase during cooling.

Graphical images for the computations of microstructure and phase transformation described in this paper can be found at http://www.math.umn.edu/~luskin and in the cited references. A more extensive description of microstructure and its computation can be found at the above website as well as in the selected references at the end of this paper.

2. Numerical Analysis of Microstructure

Martensitic crystals typically exist in metastable states for time-scales of technological interest. Many important analytic results have been obtained for mathematical models for martensitic crystals, especially for energy-minimizing deformations with microstructure [1, 2, 11, 20, 30, 35]. These results and concepts for energy-minimizing deformations should also have a role in the analysis of metastability [18, 29]. Similarly, we have developed a numerical analysis of microstructure [4, 6, 12, 14, 16, 22, 25–28] for which results have been obtained primarily for the approximation of energy-minimizing deformations that we think also give insight and some validation for the investigation of metastability by computational methods.

We give here a summary of the numerical analysis of martensitic microstructure that we have developed for temperatures $\theta < \theta_T$ for which the energy density $\phi(F,\theta)$ is minimized on the martensitic variants $\mathcal{U} = \mathrm{SO}(3)U_1 \cup \cdots \cup \mathrm{SO}(3)U_N$.

We assume that the energy density $\phi(F,\theta)$ is continuous and satisfies near the minimizing deformation gradients $\mathcal{U}$ the quadratic growth condition given by

$$\phi(F,\theta) \geq \mu \, \|F - \pi(F)\|^2 \qquad \text{for all } F \in \mathbb{R}^{3\times 3}, \tag{2.1}$$

where $\mu > 0$ is a constant and $\pi : \mathbb{R}^{3\times 3} \to \mathcal{U}$ is a projection satisfying

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

We also assume that the energy density $\phi(F,\theta)$ satisfies the growth condition for large F given by

$$\phi(F,\theta) \geq C_1 \|F\|^p - C_0 \qquad \text{for all } F \in \mathbb{R}^{3\times 3},$$

where C_0 and C_1 are positive constants independent of $F \in \mathbb{R}^{3\times 3}$ where $p > 3$ to ensure that deformations with finite energy are uniformly continuous.

We can then denote the set of deformations of finite energy by

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

and we can define the set $\mathcal{A}$ of admissible deformations to be

$$\mathcal{A} = \{\, y \in W^\phi : y(x) = y_0(x) \text{ for all } x \in \partial\Omega \,\}. \tag{2.2}$$

Since we assume that the set of admissible deformations $\mathcal{A}$ is constrained on the entire boundary $\partial\Omega$, we can neglect the loading energy in (1.1). We will also set the interfacial energy to be zero in this section so as to consider the idealized model for which the length scale of the microstructure is infinitesimally small. For the theorems below, we assume boundary conditions compatible with a simple laminate mixing QU_i for $Q \in \mathrm{SO}(3)$ with volume fraction λ and U_j with volume fraction $1-\lambda$,

$$y_0(x) = [\lambda Q U_i + (1-\lambda) U_j]\, x \qquad \text{for all } x \in \Omega,$$

where for $a \in \mathbb{R}^3$ and $n \in \mathbb{R}^3$, with $a,\, n \neq 0$, we have the interface equation [1, 19, 25]

$$QU_i = U_j + a \otimes n.$$

We consider the finite element approximation of the variational problem

$$\inf_{y \in \mathcal{A}} \mathcal{E}(y)$$

given by

$$\inf_{y_h \in \mathcal{A}_h} \mathcal{E}(y_h)$$

where $\mathcal{A}_h$ is a finite-dimensional subspace of $\mathcal{A}$ defined for $h \in (0, h_0]$ for some $h_0 > 0$. The following approximation theorem for the energy has been proven for the P_k or Q_k type conforming finite elements on quasi-regular meshes, in particular for the P_1 linear elements defined on tetrahedra and the Q_1 trilinear elements defined on rectangular parallelepipeds [4, 10, 22, 25–27].

Theorem 2.1. *For each $h \in (0, h_0]$, there exists $y_h \in \mathcal{A}_h$ such that*

$$\mathcal{E}(y_h) = \min_{z_h \in \mathcal{A}_h} \mathcal{E}(z_h) \leq Ch^{1/2}. \tag{2.3}$$

We next define the volume fraction that an admissible deformation $y \in \mathcal{A}$ is in the k-th variant $\mathrm{SO}(3)U_k$ for $k \in \{1, \ldots, N\}$ by

$$\tau_k(y) = \frac{\operatorname{meas} \Omega_k(y)}{\operatorname{meas} \Omega}$$

where

$$\Omega_k(y) = \{\, x \in \Omega : \pi(\nabla y(x)) \in \mathrm{SO}(3)U_k \,\}.$$

The following stability theory was first proven for the orthorhombic to monoclinic transformation ($N = 2$) [26] and then for the cubic to tetragonal transformation ($N = 3$) [22]. The analysis of stability is more difficult for larger N since the additional wells give the crystal more freedom to deform without the cost of additional energy. In fact, for the tetragonal to monoclinic transformation ($N = 4$) [6], the orthorhombic to triclinic transformation ($N = 4$) [16], and the cubic to orthorhombic transformation ($N = 6$) [4] we have shown that there are special lattice constants for which the laminated microstructure is not stable. Error estimates are obtained by substituting the approximation result (2.3) in the following stability results.

In each case for which we have proven the approximation of the microstructure to be stable, we have derived the following basic stability estimate for the approximation of a simple laminate mixing QU_i and U_j which bounds the volume fraction that $y \in \mathcal{A}$ is in the variants $k \neq i, j$

$$\tau_k(y) \leq C \left(\mathcal{E}(y)^{\frac{1}{2}} + \mathcal{E}(y) \right) \qquad \text{for all } k \neq i, j \text{ and } y \in \mathcal{A}. \tag{2.4}$$

For the theorems that follow, we shall assume that the lattice parameters are such that the estimate (2.4) holds.

The following theorem gives estimates for the strong convergence of the projection of the deformation gradient parallel to the laminates (the projection of the deformation gradient transverse to the laminates does not converge strongly [25]), the strong convergence of the deformation, and the weak convergence of the deformation gradient.

Theorem 2.2. *(1) For any $w \in \mathbb{R}^3$ such that $w \cdot n = 0$ and $|w| = 1$, we have the estimate for the strong convergence of the projection of the deformation gradient*

$$\int_\Omega |\, (\nabla y(x) - \nabla y_0(x))\, w|^2 \, dx \leq C \left(\mathcal{E}(y) + \mathcal{E}(y)^{\frac{1}{2}} \right) \qquad \textit{for all } y \in \mathcal{A}.$$

(2) We have the estimate for the strong convergence of the deformation

$$\int_\Omega |y(x) - y_0(x)|^2 \, dx \le C \left(\mathcal{E}(y) + \mathcal{E}(y)^{\frac{1}{2}} \right) \qquad \textit{for all } y \in \mathcal{A}.$$

(3) For any Lipshitz domain $\omega \subset \Omega$, there exists a constant $C = C(\omega) > 0$ such that we have the estimate for the weak convergence of the deformation gradient

$$\left\| \int_\omega (\nabla y(x) - \nabla y_0(x)) \, dx \right\| \le C \left(\mathcal{E}(y)^{\frac{1}{8}} + \mathcal{E}(y)^{\frac{1}{2}} \right) \qquad \textit{for all } y \in \mathcal{A}.$$

For fixed i, j with $i \neq j$ we define a projection operator $\pi_{ij} : \mathbb{R}^{3\times 3} \to \mathrm{SO}(3)U_i \cup \mathrm{SO}(3)U_j$ by

$$\|F - \pi_{ij}(F)\| = \{\|F - G\| : G \in \mathrm{SO}(3)U_i \cup \mathrm{SO}(3)U_j\} \qquad \text{for all } F \in \mathbb{R}^{3\times 3},$$

and the operators $\Theta : \mathbb{R}^{3\times 3} \to SO(3)$ and $\Pi : \mathbb{R}^{3\times 3} \to \{QU_i, U_j\}$ by the unique decomposition

$$\pi_{ij}(F) = \Theta(F)\Pi(F) \qquad \text{for all } F \in \mathbb{R}^{3\times 3}.$$

The next theorem shows that the deformation gradients of energy-minimizing sequences must oscillate between QU_i and U_j.

Theorem 2.3. *We have for all $y \in \mathcal{A}$ that*

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

We now present an estimate for the local volume fraction that a deformation $y \in \mathcal{A}$ is near QU_i or U_j. To describe this, we define the sets

$$\omega_\rho^i(y) = \{\, x \in \omega : \Pi(\nabla y(x)) = QU_i \text{ and } \|\nabla y(x) - QU_i\| \le \rho \,\},$$

$$\omega_\rho^j(y) = \{\, x \in \omega : \Pi(\nabla y(x)) = U_j \text{ and } \|\nabla y(x) - U_j\| \le \rho \,\},$$

for any subset $\omega \in \Omega$, $\rho > 0$, and $y \in \mathcal{A}$. The next theorem demonstrates that the deformation gradients of energy-minimizing sequences must oscillate with local volume fraction λ near QU_i and local volume fraction $1 - \lambda$ near U_j.

Theorem 2.4. *For any Lipshitz domain $\omega \subset \Omega$ and for any $\rho > 0$, there exists a constant $C = C(\omega, \rho) > 0$ such that for all $y \in \mathcal{A}$*

$$\left| \frac{\operatorname{meas} \omega_\rho^i(y)}{\operatorname{meas} \omega} - \lambda \right| + \left| \frac{\operatorname{meas} \omega_\rho^j(y)}{\operatorname{meas} \omega} - (1 - \lambda) \right| \le C \left(\mathcal{E}(y)^{\frac{1}{8}} + \mathcal{E}(y)^{\frac{1}{2}} \right).$$

We next give an estimate for the weak stability of nonlinear functions of deformation gradients.

Theorem 2.5. *We have for all $f : \Omega \times \mathbb{R}^{3\times 3} \to \mathbb{R}$ and $y \in \mathcal{A}$ that*

$$\int_\Omega \{f(x, \nabla y(x)) - [\lambda f(x, QU_i) + (1 - \lambda) f(x, U_j)]\} \, dx \le C \|f\|_{\mathcal{V}} \left[\mathcal{E}(y)^{\frac{1}{4}} + \mathcal{E}(y)^{\frac{1}{2}} \right]$$

where

$$\|f\|_{\mathcal{V}}^2 = \int_\Omega \left\{ (\operatorname{ess\,sup} \|\nabla_F f(x,F)\|)^2 + |\nabla z_f(x) n|^2 + z_f(x)^2 \right\} dx < \infty$$

with $z_f : \Omega \to \mathbb{R}$ *defined by*

$$z_f(x) = f(x, QU_i) - f(x, U_j) \qquad \textit{for all } x \in \Omega.$$

3. A Computational Model for Martensitic Phase Transformation

We have developed a computational model for the quasi-static evolution of the martensitic phase transformation of a single crystal thin film [8]. Our thin film model [7] includes surface energy, as well as sharp phase boundaries with finite energy. The model also includes the nucleation of regions of the high temperature phase (austenite) as the film is heated through the transformation temperature and nucleation of regions of the low temperature phase (martensite) as the film is cooled. The nucleation step in our algorithm is needed since the film would otherwise not transform.

For our total-variation surface energy model, the bulk energy for a film of thickness $h > 0$ with reference configuration $\Omega_h \equiv \Omega \times (-h/2,\, h/2)$, where $\Omega \subset \mathbb{R}^2$ is a domain with a Lipschitz continuous boundary $\partial\Omega$, is given by the sum of the surface energy and the elastic energy

$$\kappa \int_{\Omega_h} |D(\nabla u)| + \int_{\Omega_h} \phi(\nabla u, \theta)\, dx \tag{3.1}$$

where $\int_{\Omega_h} |D(\nabla u)|$ is the total variation of the deformation gradient [7] and κ is a small positive constant.

We have shown in [7] that energy-minimizing deformations u of the bulk energy (3.1) are asymptotically of the form

$$u(x_1, x_2, x_3) = y(x_1, x_2) + b(x_1, x_2)x_3 + \mathrm{o}(x_3^2) \text{ for } (x_1, x_2) \in \Omega,\ x_3 \in (-h/2,\, h/2),$$

(which is similar to that found for a diffuse interface model [3]) where (y, b) minimizes the thin film energy

$$\mathcal{E}(y, b, \theta) = \kappa \left(\int_\Omega |D(\nabla y|b|b)| + \sqrt{2} \int_{\partial\Omega} |b - b_0| \right) + \int_\Omega \phi(\nabla y|b, \theta)\, dx \tag{3.2}$$

over all deformations of finite energy such that $y = y_0$ on $\partial\Omega$. The map b describes the deformation of the cross-section relative to the film [3]. We denote by $(\nabla y|b) \in \mathbb{R}^{3\times 3}$ the matrix whose first two columns are given by the columns of ∇y and the last column by b. In the above equation, $\int_\Omega |D(\nabla y|b|b)|$ is the total variation of the vector valued function $(\nabla y|b|b) : \Omega \to \mathbb{R}^{3\times 4}$.

We describe our finite element approximation of (3.2) by letting the elements of a triangulation τ of Ω be denoted by K and the inter-element edges by e. We

denote the internal edges by $e \subset \Omega$ and the boundary edges by $e \subset \partial\Omega$. We define the jump of a function ψ across an internal edge $e \subset \Omega$ shared by two elements $K_1, K_2 \in \tau$ to be

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

where ψ_{e,K_i} denotes the trace on e of $\psi|_{K_i}$, and we define $\psi|_e$ to be the trace on e for a boundary edge $e \subset \partial\Omega$. Next, we denote by $\mathcal{P}_1(\tau)$ the space of continuous, piecewise linear functions on Ω which are linear on each $K \in \tau$ and by $\mathcal{P}_0(\tau)$ the space of piecewise constant functions on Ω which are constant on each $K \in \tau$. Finally, for deformations $(y, b) \in \mathcal{P}_1(\tau) \times \mathcal{P}_0(\tau)$ and temperature fields $\tilde{\theta} \in \mathcal{P}_0(\tau)$, the energy (3.2) is well-defined and we have that

$$\begin{aligned}
&\kappa \left[\int_\Omega |D(\nabla y|b|b)| + \sqrt{2} \int_{\partial\Omega} |b - b_0| \right] + \int_\Omega \phi(\nabla y|b, \tilde{\theta})\, dx \\
&\quad = \kappa \left(\sum_{e \subset \Omega} \Big| [\![\, (\nabla y|b|b) \,]\!]_e \Big| \, |e| + \sqrt{2} \sum_{e \subset \partial\Omega} \Big| b|_e - b_0|_e \Big| \, |e| \right) + \sum_{K \in \tau} \phi\big((\nabla y|b, \tilde{\theta})|_K\big) \, |K|,
\end{aligned}$$

where $|\cdot|$ denotes the euclidean vector norm, $|e|$ denotes the length of the edge e, $|K|$ is the area of the element K, and

$$\Big| [\![\, (\nabla y|b|b) \,]\!]_e \Big| = \Big(\big| [\![\, \nabla y \,]\!]_e \big|^2 + 2 \, \big| [\![\, b \,]\!]_e \big|^2 \Big)^{1/2}.$$

The above term is not differentiable everywhere, so we have regularized it in our numerical simulations.

Since martensitic alloys are known to transform on a fast time scale, we model the transformation of the film from martensite to austenite during heating by assuming that the film reaches an elastic equilibrium on a faster time scale than the evolution of the temperature, so the temperature $\tilde{\theta}(x, t)$ can be obtained from a time-dependent model for thermal evolution [8]. To compute the evolution of the deformation, we partition the time interval $[0, T]$ for $T > 0$ by $0 = t_0 < t_1 < \cdots < t_{L-1} < t_L = T$ and then obtain the solution $(y(t_\ell), b(t_\ell)) \in \mathcal{A}_\tau$ for $\ell = 0, \ldots, L$ by computing a local minimum for the energy $\mathcal{E}(v, c, \theta(t_\ell))$ with respect to the space of approximate admissible deformations

$$\mathcal{A}_\tau = \{(v, c) \in \mathcal{P}_1(\tau) \times \mathcal{P}_0(\tau) : \; v = y_0 \text{ on } \partial\Omega\}. \tag{3.3}$$

Since the martensitic transformation strains $\mathcal{U} \subset \mathbb{R}^{3\times 3}$ are local minimizers of the energy density $\phi(F, \theta)$ for all θ near θ_T, a deformation that is in the martensitic phase will continue to be a local minimum for the bulk energy $\mathcal{E}(v, c, \theta(t))$ for $\theta > \theta_T$. Hence, our computational model will not simulate a transforming film if we compute $(y(t_\ell), b(t_\ell)) \in \mathcal{A}_\tau$ by using an energy-decreasing algorithm with the initial state for the iteration at t_ℓ given by the deformation at $t_{\ell-1}$, that is, if $(y^{[0]}(t_\ell), b^{[0]}(t_\ell)) = (y(t_{\ell-1}), b(t_{\ell-1}))$. We have thus developed and utilized an algorithm to nucleate regions of austenite into $(y(t_{\ell-1}), b(t_{\ell-1})) \in \mathcal{A}_\tau$ to obtain an initial iterate $(y^{[0]}(t_\ell), b^{[0]}(t_\ell)) \in \mathcal{A}_\tau$ for the computation of $(y(t_\ell), b(t_\ell)) \in \mathcal{A}_\tau$.

We used an "equilibrium distribution" function, $P(\theta)$, to determine the probability for which the crystal will be in the austenitic phase at temperature θ and we

assume that an equilibrium distribution has been reached during the time between $t_{\ell-1}$ and t_ℓ. The distribution function $P(\theta)$ has the property that $0 < P(\theta) < 1$ and

$$P(\theta) \to 0 \text{ as } \theta \to -\infty \quad \text{and} \quad P(\theta) \to 1 \text{ as } \theta \to \infty.$$

At each time t_ℓ, we first compute a pseudo-random number $\sigma(K,\ell) \in (0,1)$ on every triangle $K \in \tau$, and we then compute $(y^{[0]}(t_\ell), b^{[0]}(t_\ell)) \in \mathcal{A}_\tau$ by (x_K denotes the barycenter of K):

1. If $\sigma(K,\ell) \le P\left(\theta(x_K,t_\ell)\right)$ and $(\nabla y(x_K,t_{\ell-1})|b(x_K,t_{\ell-1}),\theta(x_K,t_\ell))$ is in austenite, then set
$$(y^{[0]}(t_\ell), b^{[0]}(t_\ell)) = (y(t_{\ell-1}), b(t_{\ell-1})) \text{ on } K.$$
2. If $\sigma(K,\ell) \le P\left(\theta(x_K,t_\ell)\right)$ and $(\nabla y(x_K,t_{\ell-1})|b(x_K,t_{\ell-1}),\theta(x_K,t_\ell))$ is in martensite, then transform to austenite on K.
3. If $\sigma(K,\ell) > P\left(\theta(x_K,t_\ell)\right)$ and $(\nabla y(x_K,t_{\ell-1})|b(x_K,t_{\ell-1}),\theta(x_K,t_\ell))$ is in austenite, then transform to martensite on K.
4. If $\sigma(K,\ell) > P\left(\theta(x_K,t_\ell)\right)$ and $(\nabla y(x_K,t_{\ell-1})|b(x_K,t_{\ell-1}),\theta(x_K,t_\ell))$ is in martensite, then set
$$(y^{[0]}(t_\ell), b^{[0]}(t_\ell)) = (y(t_{\ell-1}), b(t_{\ell-1})) \text{ on } K.$$

We have shown in [8] for a thin film of a CuAlNi alloy in the "tent" configuration that we can compute the nucleation above by setting $y^{[0]}(t_\ell) = y(t_{\ell-1}) \in \mathcal{P}_1(\tau)$ and by updating the piecewise constant $b^{[0]}(t_\ell) \in \mathcal{P}_0(\tau)$ by

$$b^{[0]}(x_K,t_\ell) = \frac{y_{,1}(x_K,t_{\ell-1}) \times y_{,2}(x_K,t_{\ell-1})}{|y_{,1}(x_K,t_{\ell-1}) \times y_{,2}(x_K,t_{\ell-1})|} \qquad \text{on } K$$

to nucleate austenite and

$$b^{[0]}(x_K,t_\ell) = \gamma\,\frac{y_{,1}(x_K,t_{\ell-1}) \times y_{,2}(x_K,t_{\ell-1})}{|y_{,1}(x_K,t_{\ell-1}) \times y_{,2}(x_K,t_{\ell-1})|} \qquad \text{on } K$$

to nucleate martensite.

We then compute $(y(t_\ell), b(t_\ell)) \in \mathcal{A}_\tau$ by the Polak-Ribière conjugate gradient method with initial iterate $(y^{[0]}(t_\ell), b^{[0]}(t_\ell)) \in \mathcal{A}_\tau$. We have also experimented with several other versions of the above algorithm for the computation of $b^{[0]}(t_\ell)$. For example, the above algorithm can be modified to utilize different probability functions $P(\theta)$ in elements with increasing and decreasing temperature. We can also prohibit the transformation from austenite to martensite in an element in which the temperature is increasing or prohibit the transformation from martensite to austenite in an element for which the temperature is decreasing.

References

[1] J. Ball & R. James, Fine phase mixtures as minimizers of energy *Arch. Rat. Mech. Anal.* 100 (1987), 13–52.

[2] J. Ball & R. James, Proposed experimental tests of a theory of fine microstructure and the two-well problem, *Phil. Trans. R. Soc. Lond. A* 338 (1992), 389–450.

[3] K. Bhattacharya & R. James, A theory of thin films of martensitic materials with applications to microactuators, *J. Mech. Phys. Solids* 47 (1999), 531–576.

[4] K. Bhattacharya, B. Li, & M. Luskin, The simply laminated microstructure in martensitic crystals that undergo a cubic to orthorhombic phase transformation, *Arch. Rat. Mech. Anal.* 149 (1999), 123–154.

[5] P. Bělík, T. Brule, & M. Luskin, On the numerical modeling of deformations of pressurized martensitic thin films, *Math. Model. Numer. Anal.* 35 (2001), 525–548.

[6] P. Bělík & M. Luskin, Stability of microstructure for tetragonal to monoclinic martensitic transformations. *Math. Model. Numer. Anal. 34* (2000), 663–685.

[7] P. Bělík & M. Luskin, A total-variation surface energy model for thin films of martensitic crystals, *Interfaces and Free Boundaries* 4 (2002), 71–88.

[8] P. Bělík & M. Luskin, A computational model for the indentation and phase transformation of a martensitic thin film, *J.Mech. Phys. Solids* 50 (2002) 1789–1815.

[9] C. Carstensen & P. Plecháč, Numerical analysis of compatible phase transitions in elastic solids, *SIAM J. Numer. Anal.* 37 (2000), 2061–2081.

[10] M. Chipot, C. Collins, & D. Kinderlehrer, Numerical analysis of oscillations in multiple well problems, *Numer. Math.* 70 (1995), 259–282.

[11] M. Chipot & Kinderlehrer, D. Equilibrium configurations of crystals, *Arch. Rat. Mech. Anal.* 103 (1988), 237–277.

[12] C. Collins, D. Kinderlehrer & M. Luskin, Numerical approximation of the solution of a variational problem with a double well potential, *SIAM J. Numer. Anal.* 28 (1991), 321–332.

[13] C. Collins & M. Luskin, The computation of the austenitic-martensitic phase transition, In *Partial Differential Equations and Continuum Models of Phase Transitions* (New York, 1989), vol. 344 of *Lecture Notes in Physics*, Springer-Verlag, pp. 34–50.

[14] C. Collins & M. Luskin, Optimal order error estimates for the finite element approximation of the solution of a nonconvex variational problem, *Math. Comp.* 57 (1991), 621–637.

[15] G. Dolzmann, Numerical computation of rank-one convex envelopes. *SIAM J. Numer. Anal.* 36 (1999), 1621–1635.

[16] Y. Efendiev & M. Luskin, Stability of microstructures for some martensitic transformations, *Mathematical and Computer Modelling* 34 (2000), 1289–1305.

[17] J. Ericksen, Constitutive theory for some constrained elastic crystals, *J. Solids and Structures* 22 (1986), 951–964.

[18] R. James, Hysteresis in phase transformations, In *Proc. ICIAM-95* (1996), K. Kirchgässner, O. Mahrenholtz, and R. Mennicken, Eds., Akademie Verlag, pp. 135–154.

[19] R. James & K. Hane, Martensitic transformations and shape memory materials, *Acta Materialia* 48 (2000), 197–222.

[20] R. Kohn & S. Müller, Surface energy and microstructure in coherent phase transitions, *Comm. Pure and Appl. Math.* 47 (1994), 405–435.
[21] M. Kružík, Numerical approach to double well problems, *SIAM J. Numer. Anal.* 35 (1998), 1833–1849.
[22] B. Li & M. Luskin, Finite element analysis of microstructure for the cubic to tetragonal transformation, *SIAM J. Numer. Anal.* 35 (1998), 376–392.
[23] B. Li & M. Luskin, Theory and computation for the microstructure near the interface between twinned layers and a pure variant of martensite, *Materials Science & Engineering A* 273 (1999), 237–240.
[24] Z. Li, Rotational transformation method and some numerical techniques for computing microstructures. *Math. Models Methods Appl. Sci.* 8 (1998), 985–1002.
[25] M. Luskin, On the computation of crystalline microstructure. *Acta Numerica* 5 (1996), 191–258.
[26] M. Luskin, Approximation of a laminated microstructure for a rotationally invariant, double well energy density. *Numer. Math. 75* (1997), 205–221.
[27] M. Luskin & L. Ma, Analysis of the finite element approximation of microstructure in micromagnetics, *SIAM J. Numer. Anal.* 29 (1992), 320–331.
[28] M. Luskin & L. Ma, Numerical optimization of the micromagnetics energy, In *Mathematics in Smart Materials* (1993), SPIE, pp. 19–29.
[29] A. Mielke, F. Theil, & V. I. Levitas, A variational formulation of rate-independent phase transformations using an extremum principle. *Arch. Rat. Mech. Anal.* 162 (2002), 137–177.
[30] S. Müller, Singular perturbations as a selection criterion for periodic minimizing sequences, *Calc. Var.* 1 (1993), 169–204.
[31] R. Nicolaides & N. Walkington, Strong convergence of numerical solutions to degenerate variational problems, *Math. Comp.* 64 (1995), 117–127.
[32] P. Pedregal, On the numerical analysis of non-convex variational problems, *Numer. Math.* 74 (1996), 325–336.
[33] M. Pitteri & G. Zanzotto, *Continuum models for twinning and phase transitions in crystals*, Chapman and Hall, London, 1996.
[34] T. Roubíček, Numerical approximation of relaxed variational problems, *J. Convex Anal.* 3 (1996), 329–347.
[35] V. Šverák, Rank-one convexity does not imply quasiconvexity, *Proc. Royal Soc. Edinburgh* 120A (1992), 185–189.
[36] L. Truskinovsky & G. Zanzotto, Finite-scale microstructures and metastability in one-dimensional elasticity, *Meccanica* 30 (1995), 557–589.