

# Numerical Methods for Martensitic Phase Transformation and Microstructure

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## Abstract

Phase transformation, metastability, and microstructure offer great challenges to the development and analysis of numerical methods. We present some solutions to these problems that we have developed in the context of martensitic structural phase transformations. These crystals are observed to be in metastable states (local minima), sometimes exhibit fine-scale spatial oscillation, and hysteresis is observed as the temperature or boundary forces are varied. We present computational methods and a numerical analysis for this microstructure, and we discuss several multiscale methods and the different metastable states that they compute.

## 1 Introduction

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 [4]. 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. A more detailed discussion of our algorithm and graphical displays of computational results for our model are given in [4].

A review of mathematical and numerical methods for martensitic phase transformation and microstructure is given in [4]. A more recent study of the numerical analysis of microstructure is given in [2]. A more extensive bibliography of papers on the numerical analysis of the martensitic phase transformation and microstructure can be found at <http://www.math.umn.edu/~luskin/>.

## 2 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 [4]. Our thin film model [3] includes surface energy, as well as sharp phase boundaries with finite energy. The model also

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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

$$\kappa \int_{\Omega_h} |D(\nabla u)| + \int_{\Omega_h} \phi(\nabla u, \theta) dx \quad (8)$$

where  $\int_{\Omega_h} |D(\nabla u)|$  is the total variation of the deformation gradient [3] and  $\kappa$  is a small positive constant.

We have shown in [3] that energy-minimizing deformations  $u$  of the bulk energy (8) are asymptotically of the form

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

(which is similar to that found for a diffuse interface model [1]) where  $(y, b)$  minimizes the thin film energy

$$\mathcal{E}(y, b, \theta) = \kappa \left( \int_{\Omega} |D(\nabla y|b|b)| + \sqrt{2} \int_{\partial\Omega} |b - b_0| \right) + \int_{\Omega} \phi(\nabla y|b, \theta) dx \quad (9)$$

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 [1, 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  $\nabla y$  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  $(\nabla y|b|b) : \Omega \rightarrow \mathbb{R}^{3 \times 4}$ .

We describe our finite element approximation of (9) by letting the elements of a triangulation  $\tau$  of  $\Omega$  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  $\psi$  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  $\psi_{e, K_i}$  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  $\Omega$  which are linear on each  $K \in \tau$  and by  $\mathcal{P}_0(\tau)$  the space of piecewise constant functions on  $\Omega$  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 (9) is well-defined and we have that

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

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

$$\left| \llbracket (\nabla y | b | b) \rrbracket_e \right| = \left( \left| \llbracket \nabla y \rrbracket_e \right|^2 + 2 \left| \llbracket b \rrbracket_e \right|^2 \right)^{1/2}.$$

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 [4]. To compute the evolution of the deformation, we partition the time interval  $[0, T]$  for  $T > 0$  by  $0 = t_0 < t_1 < \dots < t_{L-1} < t_L = T$  and then obtain the solution  $(y(t_\ell), b(t_\ell)) \in \mathcal{A}_\tau$  for  $\ell = 0, \dots, L$  by computing a local minimum for the energy  $\mathcal{E}(v, c, \theta(t_\ell))$  with respect to the space of approximate admissible deformations

$$\mathcal{A}_\tau = \{(v, c) \in \mathcal{P}_1(\tau) \times \mathcal{P}_0(\tau) : v = y_0 \text{ on } \partial\Omega\}. \quad (10)$$

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

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

At each time  $t_\ell$ , 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  $\sigma(K, \ell) \leq P(\theta(x_K, t_\ell))$  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  $\sigma(K, \ell) \leq P(\theta(x_K, t_\ell))$  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  $\sigma(K, \ell) > P(\theta(x_K, t_\ell))$  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  $\sigma(K, \ell) > P(\theta(x_K, t_\ell))$  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 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

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