TECHNISCHE MECHANIK, 30, 1-3, (2010), 203 – 210
submitted: October 31, 2009

Variational model of martensitic thin films and its numerical treatment

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Following the derivation of the energy functional of martensitic thin films by Bhattacharya and James (1999) we propose a numerical approach to the relaxation theory of thin films. It is based on the approximation of the corresponding relaxed problem by a first-order laminate. Finally, computational experiments are shown.

1 Introduction

Variational models for microstructures assume that the formed structure has some optimality property. The reason for the formation of microstructures is that no exact optimum can be achieved and optimizing sequences have to develop finer and finer oscillations. A typical example is a microstructure in shape memory alloys which is closely related to the so-called shape memory effect, i.e. the ability of some materials to recover, on heating, their original shape. Such materials have a high-temperature phase called austenite and a low-temperature phase called martensite. The austenitic phase has only one variant but the martensitic phase exists in many symmetry related variants and can form a microstructure by mixing those variants (possibly also with the austenitic variant) on a fine scale. Such shape memory alloys, as e.g. Ni-Ti, Cu-Al-Ni or In-Th, have various technological applications.

Confining ourselves to the cases with negligible hysteresis behavior modeling of microstructures in shape memory alloys leads to a multidimensional vectorial variational problem, whose relaxation (i.e. suitable extension) is not yet satisfactorily understood. We study microstructures on mesoscopical level. This means we do not take care only about some macroscopic effective response of the material but our approach also provides some information about optimizing sequences. In the last decade similar mesoscopical models equipped with suitable dissipative potentials have been developed to treat materials with significant hysteresis; cf. Kružík et al. (2005); Roubíček (2000). A comprehensive survey of mathematical problems related to martensitic crystals can be found in Müller (1998).

In what follows we use the standard notation L^p for a Lebegue space of measurable maps which are integrable with the p-th power if $1 \leq p < +\infty$ or are measurable and essentially bounded if $p = +\infty$. Further, we use Sobolev spaces $W^{k,p}$ of maps which together with their derivatives up to the k-th order belong to L^p.

2 Model of the bulk material

The elastic energy of a body at a fixed temperature θ is usually modeled through

$$\int_\Omega W(\nabla y(x))\,\mathrm{d}x\ ,$$

where $\Omega \subset \mathbb{R}^3$ is the body, $y : \Omega \to \mathbb{R}^3$ denotes the deformation mapping, $W : \mathbb{R}^{3\times3} \to \mathbb{R}$ is the energy density and $\mathbb{R}^{3\times3}$ denotes the space of real matrices 3×3. To avoid locally the penetration of the body by itself we suppose that $\det \nabla y > 0$ almost everywhere in Ω. The energy density is a continuous function which is invariant under rotations in the sense that for any $R \in \mathrm{SO}(3) = \{R \in \mathbb{R}^{3\times3};\ \det R = 1,\ \ RR^t = R^tR = \mathrm{Id}\}$, Id the identity matrix 3×3, and any $F \in \mathbb{R}^{3\times3}$,

$$W(RF) = W(F)\ .$$

We assume that the energy density is normalized, so that $\min_{F\in\mathbb{R}^{3\times3}} W(F) = 0$.

Our goal is to model presence of different phases, which leads to the so-called well structure of W. If the temperature θ is below the transformation temperature θ_t then W is minimized on wells defined by M positive definite and symmetric matrices $F_1, \ldots, F_M$, $\det F_i > 0$ with the property $RF_i \neq F_j$ for any $R \in \mathrm{SO}(3)$ and $i \neq j$. At the transformation temperature W is minimized on F_i, $1 \leq i \leq M$ and on a symmetric and positive definite $F_0 \in \mathbb{R}^{3\times 3}$ defining the austenite phase. Above the transformation temperature W is minimized only on the well given by F_0. Clearly, if F is a minimizer for W then the whole well $\{RF; R \in \mathrm{SO}(3)\}$ is a minimizer, too.

Concretely, we assume that $\theta < \theta_t$, i.e.

$$W \geq 0 \ \text{ and } \ W(F) = 0 \ \text{ if and only if } \ F \in \bigcup_{i=1}^{M} \mathrm{SO}(3)F_i \ .$$

If there are $R_{ij} \in \mathrm{SO}(3)$, $1 \leq i < j \leq M$, such that $\mathrm{rank}(F_i - R_{ij}F_j) = 1$ we say that W has *rank-one* connected wells. This condition is very important. Namely, two variants F_i and F_j ($i \neq j$) can form a laminated structure with a planar interface if and only if

$$\mathrm{rank}(F_i - R_{ij}F_j) = 1 \tag{1}$$

for some rotation R_{ij}; cf. Ball and James (1988).

If a loading force with the density $f : \Omega \to \mathbb{R}^3$ acts on the body, the mechanical work done by this force equals to

$$-\int_\Omega f(x) \cdot y(x) \, \mathrm{d}x \ .$$

Altogether, the energy of the martensitic material under a deformation y is given by

$$I(y) = \int_\Omega (W(\nabla y(x)) - f(x) \cdot y(x)) \, \mathrm{d}x$$

and for the sake of simplicity we abbreviate

$$\Phi(y(x), \nabla y(x)) = W(\nabla y(x)) - f(x) \cdot y(x) \ .$$

We denote

$$\mathcal{A}_{y_0} = \left\{ y \in W^{1,p}(\Omega; \mathbb{R}^3); \ y = y_0 \text{ on } \Gamma \ , \ \det \nabla y > 0 \right\}$$

for $\Omega \subset \mathbb{R}^3$, a bounded domain, $\Gamma \subset \partial\Omega$, $y_0 \in W^{1,p}(\Omega; \mathbb{R}^3)$ a given mapping and $p > 3$. We suppose that $\mathcal{A}_{y_0} \neq \emptyset$.

We assume that stable states of the material are characterized by a minimum of the energy, which makes us formulate the following problem

$$\min \ \{I(y); \ \ y \in \mathcal{A}_{y_0}\} \ . \tag{2}$$

Early computations dealing with microstructures for a rotationally invariant stored energy density appeared in Collins and Luskin (1989). They used element-wise affine approximations of deformations, i.e., a direct finite element discretization of (2). We shall denote the infimum described by (2) as $\inf_{v \in \mathcal{A}_{y_0}} I(v) = \inf(2)$. We also assume that I is coercive on $W^{1,p}(\Omega; \mathbb{R}^3)$, that is, $\lim_{\|y\|_{W^{1,p}(\Omega;\mathbb{R}^3)} \to \infty} I(y) = +\infty$. Generally, no solution to (2) exists, i.e., I has no minimizer. In order to obtain a certain macroscopic deformation it is energetically convenient to develop spatial oscillations among various variants of martensite. Therefore we face the question what is the property of W which prevents such behavior, i.e., when a uniform deformation is always a minimizer with respect to its own boundary conditions. This condition is known as quasiconvexity.

Let us recall that a function $\tilde{f} : \mathbb{R}^{m\times n} \to \mathbb{R}$ is *quasiconvex* if for any matrix $A \in \mathbb{R}^{m\times n}$ and for any smooth function $\varphi : \tilde{\Omega} \subset \mathbb{R}^n \to \mathbb{R}^m$, $\varphi(x) = Ax$, for $x \in \partial\tilde{\Omega}$ it holds that

$$\int_{\tilde{\Omega}} \tilde{f}(\nabla \varphi(x)) \mathrm{d}x \geq \tilde{f}(A) \ \mathrm{meas} \ (\tilde{\Omega}) \ .$$

In fact, this definition is independent of the choice of a regular open domain $\tilde{\Omega} \subset \mathbb{R}^n$ such that $\mathrm{meas}(\partial\tilde{\Omega}) = 0$. It can be shown that for scalar or one-dimensional problems ($m = 1$ or $n = 1$) quasiconvexity reduces to usual convexity.

It is easy to see that we deal with W's which are not quasiconvex. This is the main reason why our problem does not have to have any solution. One naturally looks for a suitable extension (relaxation) of the problem which would ensure solvability. Dacorogna, in Dacorogna (1989), showed that we can formulate another minimization problem (relaxed problem), a solution of which is attained and whose minimum is equal to the infimum of (2). This minimization problem is called a *relaxed* problem

$$\min \left\{ I_Q(y) = \int_\Omega Q\Phi(y(x), \nabla y(x))\, \mathrm{d}x; \ , \ y \in \mathcal{A}_{y_0} \right\} , \tag{3}$$

where $Q\Phi(y,\cdot)$ is the quasiconvex envelope of $\Phi(y,\cdot)$ defined by

$$Q\Phi(y,\cdot) = \sup\{\tilde{f} \le \Phi(y,\cdot); \ \tilde{f} \text{ quasiconvex}\} .$$

In this case, I_Q is sequentially weakly lower semicontinuous and the problem (3) has a solution, that is, there is $y \in \mathcal{A}_{y_0}$ such that $I_Q(y) = \min_{v\in\mathcal{A}_{y_0}} I_Q(v) \equiv \min$ (3).

Finally, the relaxation theorem, which is due to ((Dacorogna, 1989, Sec.1)), says that under some growth conditions:
(i) inf (2)= min (3),
(ii) if $y \in \mathcal{A}_{y_0}$ is a solution to (3) then there is a minimizing sequence $\{y_k\}_{k\in\mathbb{N}} \subset \mathcal{A}_{y_0}$ converging weakly to y in $W^{1,p}(\Omega;\mathbb{R}^3)$ and $\lim_{k\to\infty} I(y_k) = I_Q(y)$ and
(iii) any minimizing sequence of (2) converges weakly to a minimizer of (3).

Quasiconvexity as a non-local property is generally very difficult to be verified except in some special situations and not many nontrivial quasiconvex functions are known. It follows that we almost never can find an analytical expression of the quasiconvex envelope of a particular function. This makes the problem of minimizing I_Q rather difficult to solve.

For this reason, it is useful to define a weaker (Šverák (1992)) kind of convexity than quasiconvexity, that is, rank-one convexity. A function $\tilde{f} : \mathbb{R}^{3\times3} \to R$ is *rank-one convex* if

$$\tilde{f}(\lambda A + (1-\lambda)B) \le \lambda\tilde{f}(A) + (1-\lambda)\tilde{f}(B) \ \text{ whenever } \operatorname{rank}(A-B) \le 1 \text{ and } 0 \le \lambda \le 1 .$$

We can also define the rank-one convex envelope $R\Phi$ of Φ. Let us recall that (see (Dacorogna, 1989, Sec.1))

$$R\Phi(y,\cdot) = \sup\{\tilde{f} \le \Phi(y,\cdot); \ \tilde{f} \text{ rank-one convex}\} ,$$

and that

$$Q\Phi \le R\Phi \le \Phi .$$

Using this envelope, we can state the following problem

$$\inf \left\{ I_R(y) = \int_\Omega R\Phi(y(x), \nabla y(x))\, \mathrm{d}x; \ y \in \mathcal{A}_{y_0} \right\} . \tag{4}$$

The rank-one convex envelope is characterized by the following proposition.

Proposition 2.1. *(see (Kohn and Strang, 1986, II), also (Dacorogna, 1989, sec. 5.1)) Let $\tilde{f} : \mathbb{R}^{3\times3} \to \mathbb{R}$ be bounded from below. Then for every $A \in \mathbb{R}^{3\times3}$,*

$$R\tilde{f}(A) = \lim_{k\to\infty} R_k\tilde{f}(A) \tag{5}$$

where $R_0\tilde{f} = \tilde{f}$ and

$$\begin{aligned} R_{k+1}\tilde{f}(A) \ &= \ \inf\Big\{\lambda R_k\tilde{f}(A_0) + (1-\lambda)R_k\tilde{f}(A_1); \ 0 \le \lambda \le 1, \\ &\qquad A = \lambda A_0 + (1-\lambda)A_1 \ , \ \operatorname{rank}(A_1 - A_0) \le 1 \Big\} \ , \ k \in \mathbb{N}\cup\{0\} . \end{aligned}$$

Hence, utilizing this characterization of the rank-one convex envelope we can state for any $k \in \mathbb{N}$

$$\inf \left\{ I_k(y) = \int_\Omega R_k\Phi(y(x), \nabla y(x))\,\mathrm{d}x;\ y \in \mathcal{A}_{y_0} \right\}, \tag{6}$$

where $R_k\Phi$ is an approximation (given in Proposition 1) of the rank-one convex envelope of Φ with respect to the second variable. Due to the relaxation theorem inf (2)=min (3)=inf (6). Of course, the minimum of I_k and I_R does not have to exist because $R_k\Phi$ and $R\Phi$ are not necessarily quasiconvex in the last variable. On the other hand, we will see that finite element discrete solutions to (6) always exist and already provide some information about minimizing sequences of the original problem (2).

Our results below show examples of Φ for which we obtain solutions to (6) for some $k \in \mathbb{N}$. This gives us an upper estimate of a solution to (4) and thus also to (2).

Let us figure out the form of $R_1\Phi(\cdot, \nabla y)$. To this end, we start with a convex combination

$$\nabla y = \lambda A_0 + (1-\lambda)A_1\ .$$

According to Proposition 2.1 it is necessary that $\mathrm{rank}(A_1 - A_0) \le 1$ or, equivalently, $A_1 - A_0 = q \otimes r$, where $q, r : \Omega \to \mathbb{R}^3$ are such that $q \otimes r \in L^p(\Omega; \mathbb{R}^{3\times 3})$, that is, $A_0 = \nabla y - (1-\lambda) q \otimes r$ and $A_1 = \nabla y + \lambda q \otimes r$. Denote

$$\begin{aligned} z(\lambda(x), y(x), q(x), r(x)) = \lambda(x)\Phi(y(x), \nabla y(x) - (1-\lambda(x))q(x)\otimes r(x)) \\ +(1-\lambda(x))\Phi(y(x), \nabla y(x) + \lambda(x) q(x) \otimes r(x))\ . \end{aligned} \tag{7}$$

Then the problem (6) for $k = 1$ reads

$$\begin{cases} \text{Minimize} & \int_\Omega z(\lambda(x), y(x), q(x), r(x))\,\mathrm{d}x \\ \text{subject to} & y \in \mathcal{A}_{y_0}\ ,\ \lambda \in L^\infty(\Omega)\ , 0 \le \lambda \le 1\ ,\ q, r \in L^p(\Omega; \mathbb{R}^3)\ . \end{cases} \tag{8}$$

3 Model of a thin film

Bhattacharya and James (1999) considered a problem of dimensional reduction of a bulk specimen. Let us have a domain $\Omega_h := \mathcal{S} \times (-\frac{h}{2}, \frac{h}{2})$ where $\mathcal{S} \subset \mathbb{R}^2$ is a smooth bounded plane. If $\{e_1, e_2, e_3\}$ is an orthonormal basis in $\mathbb{R}^3$ we suppose that e_3 is perpendicular to the plane of the film whereas e_1, e_2 lie in the film plane.

We define the plane gradient ∇_p by the following

$$\nabla_p y = y_{,1} \otimes e_1 + y_{,2} \otimes e_2\ ,$$

where $y_{,i}$ denotes the vector of derivatives of y with respect to x_i, $i = 1, 2$. Moreover, having a matrix $A \in \mathbb{R}^{3\times 3}$ we write $A := (a_1|a_2|a_3)$ if $A = a_1 \otimes e_1 + a_2 \otimes e_2 + a_3 \otimes e_3$, where $a_i \in \mathbb{R}^3$ for $i = 1, 2, 3$. They dealt with the following problem ($\kappa > 0$ is a "surface-energy" constant)

$$\text{minimize } J_h^\kappa(y) = \frac{1}{h}\int_{\Omega_h} \kappa |\nabla^2 y(x)|^2 + W(\nabla y(x))\,\mathrm{d}x \tag{9}$$

where

$$y \in \{u \in W^{2,2}(\Omega_h; \mathbb{R}^3);\ u(x) = Ax \text{ if } x \in \partial\mathcal{S} \times (-h/2, h/2)\}$$

where $A \in \mathbb{R}^{3\times 3}$ is fixed. Bhattacharya and James (1999) proved that (up to a subsequence) minimizers of J_h^κ, y^h, satisfy the following convergences as $h \to 0$: $\nabla_p^2 y^h \to \nabla_p^2 \bar{y}$ in $L^2(\Omega_1)$, $h^{-1}\nabla y^h_{,3} \to \nabla_p \bar{b}$ in $L^2(\Omega_1)$ and $h^{-2} y^h_{,33} \to 0$ in $L^2(\Omega_1)$. Moreover, $(\bar{y}, \bar{b}) \in W^{2,2}(\mathcal{S}; \mathbb{R}^3) \times W^{1,2}(\mathcal{S}; \mathbb{R}^3)$ minimize the following energy

$$J_0^\kappa(y, b) = \int_{\mathcal{S}} \kappa(|\nabla_p^2 y(x)|^2 + |\nabla_p b|^2) + W(y_{,1}(x)|y_{,2}(x)|b(x))\,\mathrm{d}S \tag{10}$$

subject to the boundary conditions $y(x_1, x_2) = a_1 x_1 + a_2 x_2$ and $b(x_1, x_2) = a_3$ if $(x_1, x_2) \in \partial\mathcal{S}$. Physically, $y : \mathcal{S} \to \mathbb{R}^3$ describes the the average deformation of the film while $b : \mathcal{S} \to \mathbb{R}^3$ describes the shear of the cross-section of the film. If κ is small we may consider the model without the surface energy, i.e., the elastic energy stored in the film is now

$$J_0(y,b) = \int_{\mathcal{S}} W(y_{,1}(x)|y_{,2}(x)|b(x))\,\mathrm{d}S\ . \tag{11}$$

If, moreover, some external forces $f : \mathcal{S} \to \mathbb{R}^3$ act on the film the total energy of the system is

$$J(y,b) = \int_{\mathcal{S}} W(y_{,1}(x)|y_{,2}(x)|b(x)) - f(x)\cdot y(x)\,\mathrm{d}S \tag{12}$$

The functional J is nonconvex and its minimizer does not have to exists in the set $W^{1,2}(\mathcal{S};\mathbb{R}^3) \times L^2(\mathcal{S};\mathbb{R}^3)$ equiped with suitable (e.g. affine) boundary conditions on y. Nevertheless, the situation is different compared to the bulk material. Consider the situation that $\mathcal{S} = \mathcal{S}_1 \cup \mathcal{S}_2 \cup \mathcal{L}$, where $\mathcal{S}_1$, $\mathcal{S}_2$ are disjoint subsets of $\mathcal{S}$ and $\mathcal{L}$ is a line interface between them and that

$$(y_{,1}|y_{,2}|b) = \begin{cases} R_iF_i & \text{in } \mathcal{S}_1 \\ R_jF_j & \text{in } \mathcal{S}_2\ , \end{cases}$$

where $R_i, R_j \in \mathrm{SO}(3)$ and F_i, F_j are zero energy deformation gradients. We further require that y is continuous in $\mathcal{S}$ while $y_{,1}$, $y_{,2}$ as well as b may suffer jumps over the interface $\mathcal{L}$. It is shown in Bhattacharya and James (1999) that in order to satisfy these requirements the following thin-film twinning equation must be satisfied

$$R_iF_i - R_jF_j = a \otimes n + c \otimes e_3\ , \tag{13}$$

where $a, n \in \mathbb{R}^3$, $n \cdot e_3 = 0$ and $c \in \mathbb{R}^3$ denotes the jump of b across the interface. The vector n is normal to the line interface. Thus, we say that martensitic variants i and j can form a linear thin-film interface if there are rotations R_i, R_j and vectors a, n, c as above that (13) holds. Notice, that this condition is much weaker compared to the bulk situation where we require that $\mathrm{rank}(R_iF_i - R_jF_j) = 1$. As a consequence, there are interfaces between martensitic variants in the thin film which cannot exist in the bulk material.

The equation (13) motivates our algorithm for minimization of the nonconvex J_0. Due to this nonconvexity minimizing sequences typically develop finer and finer oscillations in the gradient variable which generically leads to the nonexistence of a minimum. Having $(y_{,1}|y_{,2}|b)$ we look for two matrices $A_0, A_1 \in \mathbb{R}^{3\times 3}$ and $0 \le \lambda \le 1$ such that

$$(y_{,1}|y_{,2}|b) = \lambda A_0 + (1-\lambda)A_1\ ,$$

and

$$A_1 - A_0 = a \otimes n + c \otimes e_3$$

for some $a, n, c \in \mathbb{R}^3$, $n \cdot e_3 = 0$. Thus, we can write

$$A_0 = (y_{,1}|y_{,2}|b) - (1-\lambda)(a \otimes n + c \otimes e_3)$$

and

$$A_1 = (y_{,1}|y_{,2}|b) + \lambda(a \otimes n + c \otimes e_3)\ .$$

Taking $x \in \mathcal{S}$ we define the effective (partly relaxed) energy $\hat{W}$ at $(y_{,1}(x)|y_{,2}(x)|b(x))$ as

$$\begin{aligned}\hat{W}(y_{,1}(x)|y_{,2}(x)|b(x)) := \min_{\lambda,a,n,c}\ & \lambda W(y_{,1}(x)|y_{,2}(x)|b(x)) - (1-\lambda)(a \otimes n + c \otimes e_3)) \\ & +(1-\lambda)W(y_{,1}(x)|y_{,2}(x)|b(x)) + \lambda(a \otimes n + c \otimes e_3))\ ,\end{aligned} \tag{14}$$

where $n \cdot e_3 = 0$ and $0 \le \lambda \le 1$.

Remark 3.1. *One can also define $\hat{W}(a_1|a_2) = \min_{b \in \mathbb{R}^3} W(a_1|a_2|b)$ and instead of (14) calculate the first order laminate with $\hat{W}$ on $\mathbb{R}^{3\times 2}$. However, the formulation (14) is suitable in situations where $\hat{W}$ is difficult to be calculated explicitly.*

4 Numerical simulations

As the computational domain $\Omega = (0,8) \times (0,1)$ was taken and the zero Dirichlet boundary conditions on the two "sides" of the film $\Gamma_1 = \{0\} \times (0,1)$ and $\Gamma_2 = \{8\} \times (0,1)$ were considered. We used uniform triangular meshes $\mathcal{T}_d$ for a discretization parameter $d > 0$.

Analogously to (8) the first laminate is described by the energy functional

$$\begin{aligned}\bar{J}_1(y,b,a,n,c,\lambda) = \int_S [\lambda W(y_{,1}(x)|y_{,2}(x)|b(x)) - (1-\lambda)(a\otimes n + c\otimes e_3))\\ +(1-\lambda)W(y_{,1}(x)|y_{,2}(x)|b(x)) + \lambda(a\otimes n + c\otimes e_3)) - f(x)\cdot y(x)]\,\mathrm{d}S \end{aligned} \tag{15}$$

For the spatial discretization piecewise linear P_1, resp. piecewise constant P_0 elements for y, resp. for the other variables were used. Hence (d is the aforementioned discretization parameter),

$$\begin{aligned} \mathcal{U}_d &\equiv \{v \in C(\bar{\Omega}; \mathbb{R}^3) :\ v|_K \in P_1 \text{ for each } K \in \mathcal{T}_d,\ v = id \text{ on } \Gamma_1 \cup \Gamma_2\},\\ \mathcal{V}_d &\equiv \{v : \Omega \to \mathbb{R}^3 :\ v|_K \in P_0 \text{ for each } K \in \mathcal{T}_d\},\\ \mathcal{L}_d &\equiv \{v : \Omega \to \langle 0,1\rangle :\ v|_K \in P_0 \text{ for each } K \in \mathcal{T}_d\}, \end{aligned}$$

the discrete minimization problem takes the form

$$(P_d)\left\{\begin{array}{ll} \text{Minimize} & \bar{J}_1(y,b,a,n,c,\lambda)\\ \text{subject to} & y \in \mathcal{U}_d,\ b,a,c,n \in \mathcal{V}_d,\ \lambda \in \mathcal{L}_d,\ n\cdot e_3 = 0\ ,\ 0 \le \lambda \le 1 \end{array}\right.$$

In order to perform a numerical experiment, we consider the following energy density

$$W(F) = \min\left\{ \left| C - \begin{pmatrix} 1 & \epsilon & 0\\ \epsilon & 1+\epsilon^2 & 0\\ 0 & 0 & 1 \end{pmatrix} \right|^2, \left| C - \begin{pmatrix} 1 & -\epsilon & 0\\ -\epsilon & 1+\epsilon^2 & 0\\ 0 & 0 & 1 \end{pmatrix} \right|^2 \right\}$$

for a parameter $\epsilon > 0$, and $C = F^tF$ the right Cauchy–Green tensor. The wells of this stored energy density function are given by

$$F_1 = \begin{pmatrix} 1 & \epsilon & 0\\ 0 & 1 & 0\\ 0 & 0 & 1 \end{pmatrix}, \qquad F_2 = \begin{pmatrix} 1 & -\epsilon & 0\\ 0 & 1 & 0\\ 0 & 0 & 1 \end{pmatrix}.$$

First of all, note that F_1 and F_2 are rank-one connected for all $\epsilon > 0$, i.e., $\mathrm{rank}(F_1 - F_2) = 1$. On the other hand, let us notice that for no loading force (i.e. $f = 0$) and the given boundary conditions there is a unique solution $y(x) = x$ for all $x \in \Omega$, furthermore $\mathrm{Id} = \frac{1}{2}F_1 + \frac{1}{2}F_2$. That is why we chose as the initial point for the minimization $y = id$, $b = (0,0,1)^t$, $\lambda = 0.5$, $a = (2\epsilon,0,0)^t$, $n = (0,1,0)^t$, $c = (0,0,0)^t$ (it means that $A_0 = F_2$ and $A_1 = F_1$).

The minimization procedure was done with the aid of the L-BFGS-B optimization routine described in Byrd et al. (1995). Afterwards we visualize the fraction of the different martensitic phases by evaluating the following function on each element $K \in \mathcal{T}_d$

$$\gamma(K) = \sum_{l=1}^{2} \lambda_l \frac{|(A_l^K)^t A_l^K - F_1^t F_1|^2}{|(A_l^K)^t A_l^K - F_1^t F_1|^2 + |(A_l^K)^t A_l^K - F_2^t F_2|^2},$$

where $\lambda_1 \equiv \lambda$ and $\lambda_2 \equiv 1 - \lambda$. Then γ is interpolated between zero and one on the white-black color scale.

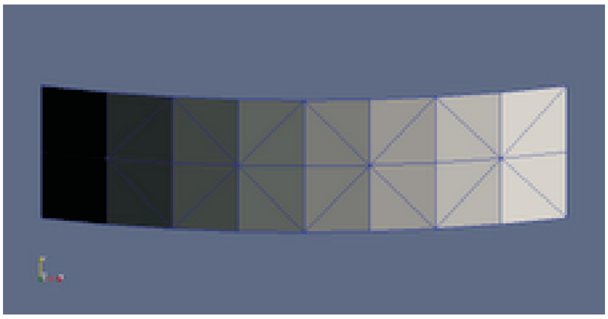

Figure 1: A thin film loaded in the y-direction. The gray color reflects the volume fraction of F_1

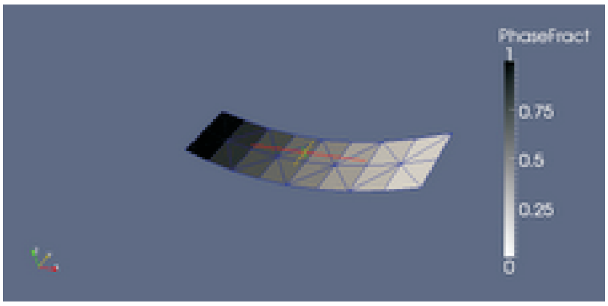

Figure 2: A thin film loaded in the y and z directions. The gray color reflects the volume fraction of F_1

5 Discussion

This paper suggests a relaxation (i.e. an extension of the notion of a solution) to a variational model of thin films where the lack of convexity typically leads to non-existence of a solution. This might be overcome by replacing the stored energy density of the material by its qusiconvexification which is, however, very rarely known. Then, typically, a partial relaxation by first or higher-order laminates is used in the numerics to capture the observed features in the bulk material. To our best knowledge, this is the first paper which specializes this technique to numerical relaxation in martensitic thin films. Numerical studies and analysis related to the minimization of the model with surface energy (10) were performed e.g. in Bělík and Luskin (2007); Bělík and Luskin (2004, 2003). This leads, however, to the situation where the existence of a solution is guaranteed by the convex higher-order term. Therefore, no relaxation is needed. On the other hand, it is not clear if laminates are the right tool for the relaxation in the thin-film model because, in general, the lamination hull differs from the quasiconvex one; cf. Šverák (1992). We exploited the thin-film twinning equation (13) derived in Bhattacharya and James (1999) in the algorithm. We see two ways how to extend the model. The first one is to design an algorithm which calculates with higher-order laminates which are also observed in real materials. The second way is to enrich the model by evolution and hysteresis properties. This is now standard in bulk materials, see e.g. Kružík et al. (2005). It was observed in Zhang (2007) that rank-one connection between the austenite and a variant of martensite in the bulk material, i.e. the validity of the bulk twinning equation (1), leads to low hysteresis in the stress/strain diagram. As the thin-film twinning equation is much less restrictive than the bulk one, it would be interesting to know if there are martensitic materials with large hysteresis in the bulk but negligible one in the thin film.

Acknowledgment: The work of MK was supported by the grants VZ6840770021 (MŠMT ČR) and IAA100750802 (GAAV).

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