Numerical Treatment of Microstructure Evolution Modeling

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This contribution proposes a "macroscopical" isothermal evolution model of a laminated martensitic microstructure in multidimensional vectorial situations. Activation and dissipation mechanisms are involved, which enables to model inelastic response of crystallic materials with a good qualitative agreement with experiments.

1 Introduction; plasticity by twinning

Plasticity in metals can be caused, beside a classical slip mechanism like in the Prandtl-Reuss model, also by twinning within a martensitic phase transformation; such plasticity is addressed in particular cases as quasi-plasticity or pseudo-elasticity [6]. The martensitic transformation in monoclinic or tetragonal crystals (cf. Figure 1a) is usually activated in much lower energies than the slip plasticity and may sometimes cause dominant effects. Typical phenomena governing the martensitic transformation are:

(A) activation, i.e. the phase transformation requires sufficiently high energy;

(B) dissipation, i.e. considerable amount of energy is dissipated within the phase transformation;

(C) geometric relations, i.e. rank-one connections between adjacent twins are energetically preferred.

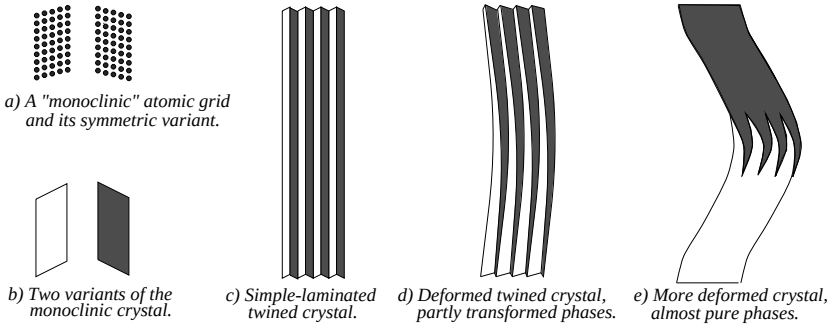

Fig. 1. Martensitic phases, twinning, phase transformation.

This contribution is an attempt to modeling of such martensitic transformation in simple vectorial cases in single crystals where the microstructure is laminated as in Figure 1c, reflecting all the phenomena (A–C). In a scalar case, a macroscopical model reflecting (A) and (A–B) has been proposed and numerically tested in [10,11] and [13], respectively.

Unfortunately, a rigorous mathematical analysis of the proposed "macroscopical" model does not seem easy and thus only rather heuristical considerations will be presented here, together with numerical experiments. It should be emphasized that, by authors' knowledge, except to some extent [1], there is no other model reflecting (A–C) in the literature, so far. For other macroscopical models of phase transformation we refer e.g. to [9,15], while "microscopical models" can be found in [2,4,5,7,14] and references therein.

2 A steady-state model of twinning

A steady-state configuration of solids is standardly considered as governed by a minimum-energy principle, say

$$\left.\begin{array}{lll} \text{Minimize} & \Phi(\nabla u)-\langle f,u\rangle & \text{for } u\in W^{1,p}(\Omega;\mathbb{R}^m),\quad u|_\Gamma=u_0 \\ \text{with} & \Phi(y):=\int_\Omega W(x,y(x))\,\mathrm{d}x\ , & \langle f,u\rangle:=\int_\Omega f(x)\cdot u(x)\,\mathrm{d}S, \end{array}\right\} \tag{1}$$

where $\Omega\subset\mathbb{R}^n$ is the reference shape of the body in question with a boundary $\partial\Omega$, $\Gamma\subset\partial\Omega$, $u_0:\Gamma\to\mathbb{R}^m$ is prescribed, $u:\Omega\to\mathbb{R}^m$ is an unknown displacement, $W^{1,p}(\Omega;\mathbb{R}^m)$ is the Sobolev space of functions $u:\Omega\to\mathbb{R}^m$ having its distributional gradient ∇u in the Lebesgue space $L^p(\Omega;\mathbb{R}^{m\times n})$, and $W:\Omega\times\mathbb{R}^{m\times n}\to\mathbb{R}$ is a potential stored energy density and $f\in L^{np/(np-n+p)}(\Omega;\mathbb{R}^m)$ (for $p>n$) is an external body force. We refer e.g. to Ball and James [3], or also to [12; Chapter 6].

In a large class of "smart" materials (as shape-memory alloys), $W(x,\cdot)$ is typically not convex (or, more precisely, even not quasiconvex). This may cause non-existence of any minimizer in (1), which is reflected in reality by fast spatial oscillations of ∇u called a "fine structure" or "microstructure", cf. Figure 1cd. From a macroscopical viewpoint (or, mathematically, in the limit) these fast oscillations of ∇u can be described by a probability measure ν_x on $\mathbb{R}^{m\times n}$ possibly depending (i.e. being parameterized) on $x\in\Omega$; cf. e.g. [3,12]. If also $(x\mapsto\nu_x)$ belongs to the Banach space of essentially bounded weakly measurable Radon-measure-valued mappings $L^\infty_{\rm w}(\Omega;{\rm rca}(\mathbb{R}^{m\times n}))$, then $\nu=\{\nu_x\}_{x\in\Omega}$ is called a Young measure. Moreover, we denote by $\mathcal{G}^p(\Omega;\mathbb{R}^{m\times n})$ the set of Young measures attainable by gradients of bounded sequences in $W^{1,p}(\Omega;\mathbb{R}^m)$, i.e.

$$\mathcal{G}^p(\Omega;\mathbb{R}^{m\times n}) := \Big\{\ \nu\in L^\infty_{\rm w}(\Omega;{\rm rca}(\mathbb{R}^{m\times n}));\qquad\qquad (2)$$
$$\exists\{u_k\}\subset W^{1,p}(\Omega;\mathbb{R}^m)\ \text{bounded}\quad \forall h\in C(\Omega\times\mathbb{R}^{m\times n}):$$
$$\lim_{k\to\infty}\int_\Omega h(x,\nabla u_k){\rm d}x=\int_\Omega\int_{\mathbb{R}^{m\times n}} h(x,A)\nu_x({\rm d}A){\rm d}x\ \Big\}$$

For $\bar\Phi(\nu):=\int_\Omega\int_{\mathbb{R}^{m\times n}} W(x,A)\nu_x({\rm d}A){\rm d}x$ defining the continuous extension of Φ, we can write the relaxed (i.e. continuously extended) problem as follows:

$$\left.\begin{array}{ll}\text{Minimize} & \bar\Phi(\nu)-\langle f,u\rangle\quad\text{for}\quad (u,\nu)\in Q,\\ \text{where} & Q:=\big\{\ (u,\nu)\in W^{1,p}(\Omega;\mathbb{R}^m)\times\mathcal{G}^p(\Omega;\mathbb{R}^{m\times n});\\ & u|_\Gamma=u_0,\quad \nabla u(x)=\int_{\mathbb{R}^{m\times n}} A\nu_x({\rm d}A),\quad \text{for a.a. } x\in\Omega\ \big\}.\end{array}\right\}\quad (3)$$

In general, (1) need not possesses a solution but (3) always has it if W is coercive and has a p-growth for some $p>1$ in the sense

$$\exists C\ge c>0:\qquad c|A|^p\le W(x,A)\le C(1+|A|^p).\qquad (4)$$

Then also $\inf(1)=\min(3)$ so that (3) is a correct relaxation of (1); cf. [12; Section 6.3] for more details. It may happen that (3) has a solution while (1) has not, cf. e.g. Section 4 even for $f=0$.

3 Evolution

If the external force $f=f(t)$ varies in time, the configuration (u,ν) will certainly evolve. This is, so far, a little understood process however. The potential barrier between the martensitic phases is usually very high so that it cannot be overcome by a kinetic energy even in microscopical volumes. In fact, microstructural transformation is rather activated by (a sufficiently large) temperature or stress already in much lower energies than this potential barrier. Thermally activated phase transformation is allowed due to chaotic oscillations of atoms, cf. [6]. Here we will consider only stress-activated transformation which is conjectured due to dislocation mechanism: each real crystal contains a lot of dislocations in its atomic grid that can move quite easily thorough the body with a high speed, changing one phase into the other in one atomic layer. Thus the Young measure ν, which describes from the macroscopical viewpoint this portion of phases, will then depend on time.

If we want to define the evolution $t\mapsto q(t)\equiv(u(t),\nu(t))$, we must postulate the impulse $\dot q\equiv(\dot u,\dot\nu)$ with the dot indicating the time derivative, for which

we need some geometry. Following [10,11], in [13] the geometry induced from the linear space $W^{1,p}(\Omega;\mathbb{R}^m) \times L^\infty_{\rm w}(\Omega;{\rm rca}(\mathbb{R}^{m\times n}))$ was taken and then the Rayleigh dissipation energy, being standardly a quadratic form in $\dot q$ (depending here also on q), was taken as:

$$R(q,\dot q) := \int_\Omega \frac{\left|\int_{\mathbb{R}^{m\times n}} \lambda(A)\dot\nu_x({\rm d}A)\right|^2}{\int_{\mathbb{R}^{m\times n}} a(A)\nu_x({\rm d}A)}{\rm d}x \qquad \text{with } q\equiv(u,\nu),\ \ \dot q\equiv(\dot u,\dot\nu), \quad (5)$$

where $a:\mathbb{R}^{m\times n}\to\mathbb{R}^+$ and $\lambda:\mathbb{R}^{m\times n}\to\mathbb{R}^k$ define an activation and a dissipation mechanisms, respectively; cf. (13) and (14) below.

Moreover, it is natural to define the kinetic energy as the quadratic form in terms of displacement only, i.e. $T(\dot q)\equiv T(\dot u) := \frac12\int_\Omega \varrho(x)|\dot u|^2{\rm d}x$ where $\varrho>0$ is the mass density.

In [13] the following semi-implicit time-discrete scheme has been proposed for $m=1$ (and numerically tested for $n=1$):

$$\left.\begin{aligned}\text{Minimize}\quad & \frac{1}{\tau^2}T(u^k-2u^{k-1}+u^{k-2})+\frac{1}{\tau}R(q^{k-1},q^k-q^{k-1})\\ & +\bar\Phi(\nu^k)-\frac{1}{\tau}\int_{(k-1)\tau}^{k\tau}\langle f(t),u^k\rangle{\rm d}t \qquad \text{for}\quad q^k\equiv(u^k,\nu^k)\in Q,\end{aligned}\right\} \quad (6)$$

for $k=1,2,...$ and $\tau>0$ a given time-step, with the initial conditions

$$q^0=q_0,\qquad q^{-1}=q_0-\tau p_0, \quad (7)$$

for a given initial configuration q_0 and initial impulse p_0. Standardly, we define the approximate solution $q_\tau\equiv(u_\tau,\nu_\tau)$ as piecewise affine interpolation in time between the particular values q^k. Existence of this semi-discrete solution for any $\tau>0$ can be proved similarly as in [10] by compactness arguments together with nonconcentration arguments as in [12].

If $m=1$ (i.e. the case considered in [10,11,13]), the set Q defined in (3) is convex, and then the scheme (6)–(7) is to approximate the initial-value problem for the following second-order inclusion for $q=q(t)\in Q$:

$$T'(\frac{{\rm d}^2q}{{\rm d}t^2})+R'_{\dot q}(q,\frac{{\rm d}q}{{\rm d}t})+\bar\Phi'(q)\ni\bar f-N_Q(q),\qquad q(0)=q_0,\qquad \frac{{\rm d}q}{{\rm d}t}(0)=p_0, \quad (8)$$

where $\bar f(q)\equiv\bar f(u,\nu)=\langle f,u\rangle$, $N_Q(q)$ is the normal cone at q to Q, and T' and $R'_{\dot q}$ and $\bar\Phi'$ denotes the Gâteaux differential of $T(\dot q)\equiv T(\dot u)$ and $R(q,\cdot)$ and $\bar\Phi(q)\equiv\bar\Phi(\nu)$, respectively; cf. [10,11] for the case $R(q,\dot q)$ independent of q while for a general case additional higher-order regularizing terms need to be included into the scheme to ensure the convergence $q_\tau\to q$.

Unfortunately, if $\min(m,n) > 1$, i.e. in vectorial multidimensional situations, the set of admissible configurations Q is not convex. Nevertheless, we can formally apply the scheme (6)–(7) in this case, too. The existence of a minimizer of (6) and thus a semi-discrete solution q_τ to (6)–(7) can be shown by the same compactness arguments as in case $m = 1$.

In view of (6), $q^k \in Q$ satisfies also

$$T'\left(\frac{q^k - 2q^{k-1} + q^{k-2}}{\tau^2}\right) + R'_{\dot q}\left(q^{k-1}, \frac{q^k - q^{k-1}}{\tau}\right) + \bar\Phi'(q^k) \in \frac{1}{\tau}\int_{(k-1)\tau}^{k\tau} f(t)\,\mathrm{d}t - N_Q(q^k) \tag{9}$$

with $N_Q(q)$ denoting now the Clarke normal cone at q to the nonconvex set Q. The formula (9) indicates that the continuous model might be governed by the evolution inclusion of the type (8) with $N_Q(q)$ understood in this Clarke's sense. Of course, no sort of uniqueness can now be expected because, as in usual large-deformation elasticity, various bifurcations can certainly occur.

4 Computational experiments with first-order laminates

We justified the above model on a 2-dimensional example, i.e. $m = n = 2$. As the evolution of a general microstructure is in reality extremely complicated, like in [1] we confined ourselves to first-order laminates as in Figure 1cd, i.e. each ν_x is composed only from two atoms $A_1(x), A_2(x) \in \mathbb{R}^{m\times n}$ corresponding to (deformed) particular martensitic phases from Figure 1b so that

$$\nu_x = c(x)\delta_{A_1(x)} + (1 - c(x))\delta_{A_2(x)}\,, \qquad c \in [0,1], \tag{10}$$

where δ_A is the Dirac distribution supported at the matrix A. Then, as $\nu \in \mathcal{G}^p(\Omega;\mathbb{R}^{2\times 2})$, necessarily $\mathrm{Rank}(A_1(x) - A_2(x)) \le 1$ for a.a. $x \in \Omega$, cf. [3].

Like in Figure 1c, the reference domain (i.e. undeformed body) Ω was considered as the rectangle $(0,6)\times(0,1)$. On $\Gamma := (\{0\}\times(0,1)) \cup (\{6\}\times(0,1))$ we prescribed the Dirichlet boundary condition $u|_\Gamma = u_0$ with $u_0(x) := x$. (Due to the symmetry of problems solved below, we performed the calculations in fact only on a half of Ω, and then we verified the results on the whole mesh.)

As to the material, we considered a homogeneous case (i.e. W, a, and λ independent of x) with two "monoclinic" martensitic phases (cf. Figure 1b) described by two rank-one connected orbits

$$\mathrm{SO}(2)\begin{pmatrix}1 & 0.1\\ 0 & 1\end{pmatrix} \qquad \text{and} \qquad \mathrm{SO}(2)\begin{pmatrix}1 & -0.1\\ 0 & 1\end{pmatrix}\,, \tag{11}$$

where SO(2) denotes the special orthogonal group $\{A \in \mathbb{R}^{2\times 2};\ A^{\mathrm{T}}A = \mathrm{Id} = AA^{\mathrm{T}},\ \det A = 1\}$, and a related frame-invariant potential

$$W(x,A) := \left|A^{\mathrm{T}}A - \begin{pmatrix} 1 & -0.1 \\ -0.1 & 1.01 \end{pmatrix}\right|^2 \left|A^{\mathrm{T}}A - \begin{pmatrix} 1 & 0.1 \\ 0.1 & 1.01 \end{pmatrix}\right|^2, \qquad (12)$$

where $|A| = \sum_{i=1,2}\sum_{j=1,2}[A]_{ij}^2$, see also [8] or [12; Example 6.6.4]. Note that the orbits (11) are minima of $W(x,\cdot)$. The functions λ and a from the Rayleigh dissipation energy (5) were taken as

$$\lambda(x,A) := \begin{cases} -10 & \text{if} \quad [A^{\mathrm{T}}A]_{12} < -0.01 \\ 10\cdot\sin 50\pi[A^{\mathrm{T}}A]_{12} & \text{if} \quad [A^{\mathrm{T}}A]_{12} \in [-0.01, 0.01] \\ 10 & \text{if} \quad [A^{\mathrm{T}}A]_{12} > 0.01\ . \end{cases} \qquad (13)$$

$$a(x,A) := \alpha(W(x,A)) \quad \text{with} \quad \alpha(w) := 0.01 + 10^7 \max(0, w - 0.0001)\ . \qquad (14)$$

Note that λ is constant in neighborhoods of the particular orbits from (11). The kinetic energy T (as well as p_0 in (7)) was neglected, which is well possible in many real processes except extremely quick ones, like impacts of missiles on targets etc.

To discretize the problem, we considered triangulations $\{\mathcal{T}_h\}_{h>0}$ of Ω consisting of elements K with a diameter less than $h > 0$, cf. Figure 2 bottom. To discretize the scheme (6)–(7), we restricted the minimization problem in (6) on element-wise constant two-atomic Young measures ν (and thus also on element-wise affine displacements u), i.e. we replaced the set Q by the set

$$\big\{(u,\nu)\in Q;\ \ (10) \text{ holds with } c, A_1, A_2 \text{ constant on each } K,\ K\in\mathcal{T}_h\big\}\,. \qquad (15)$$

We calculated responses for the cyclical loading regime taking $f = f(t) \equiv (f_1(t), 0)$ as displayed on Figure 2. For the initial conditions (7) we take

$$q_0 = (u^0, \nu^0) \quad \text{with} \quad u^0(x) = x\ , \quad \nu_x^0 = \frac{1}{2}\delta_{A_1} + \frac{1}{2}\delta_{A_2}\ , \quad A_{1,2} = \begin{pmatrix} 1 & \pm 0.1 \\ 0 & 1 \end{pmatrix}.$$

All of the computations were made on SGI Challenge L 4/R10000 in double precision.

To display portion of phases on each element in Figure 2 bottom, the shade of the grey color was calculated according to the weight c from (10), identifying the particular phases by means of a distance of A_l from the orbits (11).

The deformation is displayed as the displacement of the right-hand node in the center of Ω. The stress identified with f_1. Finally, the averaged portion of phases is evaluated as the average of shades over the lower half of the body.

A response of the stress, deformation and the averaged portion of phases within the cyclical loading f is displayed on Figure 2 top.

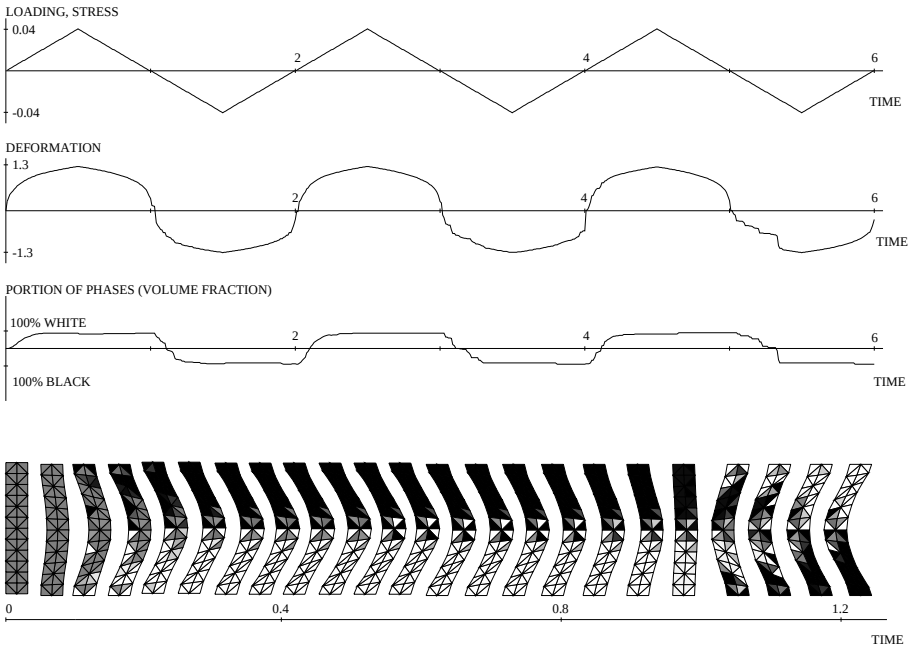

Fig. 2. Cyclical loading and the responses as functions of time.

The diagrams stress/deformation/portion of phases displayed on Figure 3 exhibit markable hysteresis effects typical in plasticity, cf. also [6].

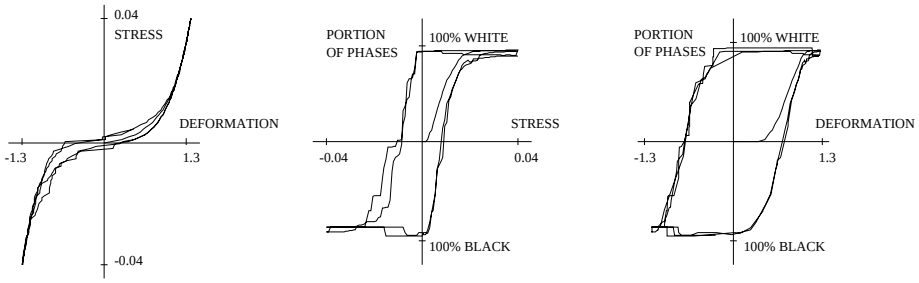

Fig. 3. Hysteresis effects corresponding to the loading regime from Figure 2.

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