

## MODELS OF MARTENSITIC TRANSFORMATION IN SHAPE-MEMORY ALLOYS

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**ABSTRACT:** Models of shape-memory alloys can be based on a continuum-mechanical description of the stored energy (having a multi-well character giving rise to microstructures) and of the dissipated energy (giving rise to hysteresis in stress/strain response). The multi-well stored energy is related to austenite and particular martensitic variants. The dissipation potential has a homogeneous degree-1 term, corresponding to (possibly rate-independent) activated processes. The configuration can be described either conventionally in terms of mere displacements or by displacements combined with special gradient Young measures to reflect better a multiscale character of the problem. Basic mathematical and numerical analysis accompany both sort of models. Isothermal computational 3D simulations with NiMnGa or CuAlNi single crystals have been done by such models. Anisothermal extension are possible in the former class of models. Selected preprints available at <http://www.karlin.mff.cuni.cz/~roubicek/multimat.htm>

### 1 INTRODUCTION, MENAGERIE OF MODELS

*Shape-memory alloys* (=SMAs) belong to so-called smart materials which enjoy important applications. SMAs exhibit specific, *hysteretic* stress/strain/temperature response and a so-called *shape-memory effect*. The mechanism behind it is quite simple: atoms tend to be arranged in several crystallographical configuration having different symmetry groups: higher symmetrical one (referred to as the *austenite* phase, typically cubic) has higher thermal capacity while lower symmetrical one (called the *martensite* phase, typically tetragonal, orthorhombic, or monoclinic) has lower thermal capacity and may exist, by symmetry, in several variants (typically 3, 6, or 12, respectively). We refer to [5, 30] for a thorough survey.

In contrast to atomistic models, this exposition focuses on models that departs from the *continuum-thermomechanics* description where the state of material is described by the

displacement and temperature, yielding a coupled system of partial-differential equations or inequalities.

Other models involve further internal variables like volume fractions etc. A particular class of such models exploits configurations described unconventionally in terms of displacements combined with special gradient Young measures to reflect better a multiscale character of the problem. For a survey of various other models, see [34].

## 2 CONTINUUM THERMODYNAMICS OF SMA<sub>s</sub>

We consider a bounded Lipschitz domain  $\Omega \subset \mathbb{R}^3$  as a reference configuration (canonically the stress-free austenite). The state variables will be the *displacement*  $u : \Omega \rightarrow \mathbb{R}^3$  and *temperature*  $\theta : \Omega \rightarrow \mathbb{R}$ ; then  $y : \Omega \rightarrow \mathbb{R}^3$  defined as  $y(x) = x + u(x)$ ,  $x \in \Omega$ , denotes the *deformation*. Hence the *deformation gradient* equals  $F = \nabla y = \mathbb{I} + \nabla u$ , where  $\mathbb{I} \in \mathbb{R}^{3 \times 3}$  denotes the identity matrix. Thermomechanical response is phenomenologically described by a specific *free energy*  $\hat{\psi} = \hat{\psi}(F, \theta)$ . The *frame-indifference*, i.e.  $\hat{\psi}(F, \theta) = \hat{\psi}(RF, \theta)$  for any  $R \in \text{SO}(3)$ , the group of orientation-preserving rotations, requires that  $\hat{\psi}(\cdot, \theta)$  in fact depends only on the (right) Cauchy-Green stretch tensor  $C := F^T F$ . Often,  $\hat{\psi}$  is considered in a simplified form, partly decoupled and linearized around a reference temperature  $\theta_r$  (=usually the equilibrium temperature between austenite and martensite), namely:

$$\hat{\psi}(F, \theta) := \hat{\phi}_0(F) + (\theta - \theta_r)\hat{\phi}_1(F) - c\theta \ln\left(\frac{\theta}{\theta_r}\right), \quad (1)$$

with frame-invariant  $C^1$ -functions  $\hat{\phi}_0, \hat{\phi}_1 : \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R}$  and with  $c > 0$  a fixed *heat capacity*. We abbreviate

$$\psi(\cdot, \theta) := \hat{\psi}(\mathbb{I} + \cdot, \theta), \quad \phi_0(\cdot) := \hat{\phi}_0(\mathbb{I} + \cdot), \quad \phi_1(\cdot) := \hat{\phi}_1(\mathbb{I} + \cdot). \quad (2)$$

The overall free energy related to a profile of  $u$  and  $\theta$  is considered as

$$\Psi(u, \theta) := \int_{\Omega} \psi(\nabla u, \theta) + \frac{\mu}{2} |\nabla^m u|^2 \, dx \quad (3)$$

where  $\mu > 0$  denotes the *capillarity*-like coefficient and  $m \geq 2$  is an integer. A certain justification of higher-order capillarity/viscosity was done, as so-called *multipolar materials*, in [24, 38]. The Gibbs' relation then defines specific *entropy*

$$s = -\frac{\partial \psi}{\partial \theta} = c \left(1 + \ln\left(\frac{\theta}{\theta_r}\right)\right) - \phi_1(F) \quad (4)$$

and the *entropy equation* is then

$$\theta \frac{\partial s}{\partial t} - \text{div}(\kappa \nabla \theta) = \xi \quad (5)$$

where  $\kappa > 0$  denotes the *heat conductivity* and  $\xi$  is a *dissipation rate* to be still specified. This represents another phenomenology in the model, reflecting e.g. various impurities and dislocations in the atomic grid that may influence dissipation, as advocated, beside [1, 16, 19, 31, 32, 34, 36, 37], essentially also e.g. in [3, 9, 11, 12, 33, 40, 42]. We consider  $\xi$  as

$$\xi := \delta_{K(\theta)}^* \left( \frac{\partial \mathcal{L}(\nabla u)}{\partial t} \right) + \mu_v(\theta) \left| \nabla^n \frac{\partial u}{\partial t} \right|^2 \quad (6)$$

where  $\mathcal{L} := \widehat{\mathcal{L}}(\mathbb{I} + \cdot)$  is a bounded  $C^1$ -function resulted from a frame-indifferent function  $\widehat{\mathcal{L}} : \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R}^L$  which distinguishes particular phases or phase variants from each other,  $\delta_{K(\theta)}^*$  the conjugate to the indicator function  $\delta_{K(\theta)}$  of a convex bounded set  $K(\theta) \subset \mathbb{R}^L$  determining (possibly temperature-dependent) *stresses to activate* particular phase transformations or, equally, the specific *energies dissipated* by them; the term  $\delta_{K(\theta)}^*$  is *degree-1 homogeneous* and is related with the *activated character of phase transformations*; we refer to the original concept [34, Formula (33)] further developed in [1, 16, 31, 32, 35] for more details. This term in (6) thus allows for reflecting the concept that the energy dissipated during transformation process depends (counting phenomenologically, beside possible rank-one connections, with various impurities) on the departing and the final (phase)variants only; this (simplifying) concept has been adopted also in [14, 29, 40, 41, 42].

Further,  $\mu_\nu = \mu_\nu(\theta) \geq \nu_0 > 0$  in (6) is a (possibly temperature-dependent) *viscosity coefficient*, and  $n \geq 2$  is an integer. The dissipation rate  $\xi$  plays the role of a (pseudo)*potential of dissipative forces* and then, by the Hamilton principle extended for dissipative systems and involving the Lagrangean  $L_\theta(u, \frac{\partial u}{\partial t}) := \Psi(u, \theta) - \frac{\rho}{2} \int_\Omega |\frac{\partial u}{\partial t}|^2 dx$ , one derives the evolution equation for  $u$  in the form

$$\rho \frac{\partial^2 u}{\partial t^2} - \operatorname{div} \left( \sigma_p + \phi'_0(\nabla u) + (\theta - \theta_r) \phi'_1(\nabla u) \right) + \mu_\nu (-1)^n \Delta^n \frac{\partial u}{\partial t} + \mu (-1)^m \Delta^m u = f \quad (7)$$

where  $\rho > 0$  is the mass density,  $f$  the external volume forces, and  $\sigma_p$  the so-called *back stress* which is to satisfy the inclusion

$$\sigma_p \in \partial \delta_{K(\theta)}^* \left( \frac{\partial}{\partial t} \mathcal{L}(\nabla u) \right) \mathcal{L}'(\nabla u) \quad \text{or equally} \quad \sigma_p \in N_{K(\theta)} \left( \mathcal{L}'(\nabla u) : \nabla \frac{\partial u}{\partial t} \right) \mathcal{L}'(\nabla u) \quad (8)$$

where “ $\partial$ ” stands for the subdifferential and  $N_K$  for the normal cone to  $K$ . By standard thermodynamical procedure, (5) with (6) yields the *heat equation* for temperature

$$c \frac{\partial \theta}{\partial t} - \operatorname{div}(\kappa \nabla \theta) = \delta_K^* \left( \mathcal{L}'(\nabla u) : \nabla \frac{\partial u}{\partial t} \right) + \mu_\nu \left| \nabla^n \frac{\partial u}{\partial t} \right|^2 + \theta \phi'_1(\nabla u) : \nabla \frac{\partial u}{\partial t} \quad (9)$$

where the right-hand side contains, beside  $\xi$  from (6), also the *adiabatic heat*  $\theta \phi'_1(\nabla u) : \nabla \frac{\partial u}{\partial t}$ ; this just gives the correct energy balance, see (15) below. Also, (9) is compatible with the non-negativity of temperature and then, at least formally in an isolated system, the *Clausius-Duhem inequality* holds:

$$\frac{d}{dt} \int_\Omega s dx = \int_\Omega \operatorname{div} \left( \kappa \frac{\nabla \theta}{\theta} \right) + \kappa \frac{|\nabla \theta|^2}{\theta^2} + \frac{\xi}{\theta} dx = \int_\Omega \kappa \frac{|\nabla \theta|^2}{\theta^2} + \frac{\xi}{\theta} dx \geq 0. \quad (10)$$

Existence of a weak solution of a initial-boundary-value problem for the overall coupled system (7)–(9) was proved in [36] for the case  $n \geq m$ ,  $n \geq 3$  with  $\mu_\nu$  and  $K$  independent of  $\theta$ . Generalization of  $\mu_\nu$  and  $K$  continuously dependent on temperature is relatively routine. Making sophisticated a-priori estimate of  $\nabla \theta \in L^{5/4-\epsilon}(Q; \mathbb{R}^3)$  simultaneously for meachanical and heat part would allow even for  $n \geq 2$ .

Models with  $K = \{0\}$  (i.e.  $\sigma_p = 0$ ) and  $\mu, \mu_\nu > 0$ ,  $n = 1$ ,  $m = 2$  was studied in [13, 25, 26, 27]. Models with no viscosity-like term, i.e.  $\mu_\nu = 0$ , have been studied in [10, 39], cf. also [6, Chap.5].

### 3 ISOTHERMAL EVOLUTION OF SHAPE-MEMORY ALLOYS

The isothermal variant of the above model, i.e. (7)–(8) with  $\theta$  constant and (9) omitted, is justified only for infinitesimally slow processes where the released/absorbed heat during the

PTs can be stabilized through the environment to keep temperature constant. Although this severe restrictions, isothermal models received substantial attention mainly because of their higher amenability for theoretical analysis than anisothermal ones.

First existence results for (7)–(8) are in [31]. Vanishing-viscosity analysis has been made in [32]. For  $K = \{0\}$  (i.e.  $\sigma_p = 0$ ), it was shown in [32] that, if  $m \geq 2$  and  $\mu_v \rightarrow 0$ , the corresponding weak solutions  $u_{\mu_v}$  converge (in terms of subsequences) to a solution  $u$  of the inviscid hyperbolic system (7) with  $\mu_v = 0$ . Such inviscid models have been studied in [10, 39], cf. also [6, Chap.5]. Moreover, [32] shows that, if  $m \geq 3$ , then even  $\int_0^T \int_{\Omega} \xi_{\mu_v} dx dt = \int_0^T \int_{\Omega} \mu_v |\nabla^n \frac{\partial}{\partial t} u_{\mu_v}| dx dt \rightarrow 0$ , i.e. the system with the capillarity term stops dissipating energy for infinitesimally small viscosity. Again, as in Sect. 2, phenomenological modelling of hysteretic response can be just made by the back stress  $\sigma_p$  from (8) and then, if  $m \geq 3$ , the solutions  $u_{\mu_v}$  to (7)–(8) converge for  $\mu_v \rightarrow 0$  (in terms of subsequences) to a solution  $u$  of the inviscid hyperbolic system (7)–(8).

Numerical simulation with such model of tension/compression experiments with NiMnGa single-crystals undergoing cubic/tetragonal transformation has been performed in [1].

## 4 MICROSTRUCTURES, YOUNG-MEASURES

Considering  $\theta$  constant as in Sect. 3 and an abstract loading  $F = F(t)$  acting on  $u$ , due to the multiwell character of  $\varphi(\cdot) = \psi(\cdot, \theta)$  and (here unspecified) boundary conditions in singlecrystals or intergranular interactions in polycrystals, the deformation gradient  $\nabla u$  of configurations minimizing the stored energy  $\Phi_{\mu}(t, u) = \Psi(u, \theta) - \langle F(t), u \rangle$  with  $\Psi$  from (1) usually tends to develop fast spatial oscillations if  $\mu \rightarrow 0$  (by scaling arguments it means in large bulks) like minimizing sequences of  $\Phi_0$  do, see [4, 5]. This results to a *microstructure* that can effectively be described by so-called *gradient Young measures*, which are measurably parameterized probability measures  $x \mapsto \nu_x$  on  $\mathbb{R}^{3 \times 3}$  that can be attained by gradients in the sense that  $\lim_{k \rightarrow \infty} \int_{\Omega} g(x) v(\nabla u_k) = \int_{\Omega} g(x) \int_{\mathbb{R}^{3 \times 3}} v(A) \nu_x(dA) dx$  for some sequence  $\{y_k\}_{k \in \mathbb{N}} \subset W^{1,p}(\Omega; \mathbb{R}^3)$  and all  $g \in L^{\infty}(\Omega)$  and  $v \in C_0(\mathbb{R}^{3 \times 3})$ , see [28]. Let us denote the set of all such parameterized measures by  $\mathcal{G}^p(\Omega; \mathbb{R}^{3 \times 3})$ . The naturally extended (so-called *relaxed*) stored energy is then

$$\bar{\Phi}(t, u, \nu) = \int_{\Omega} \int_{\mathbb{R}^{3 \times 3}} \varphi(A) \nu_x(dA) dx - \langle F(t), u \rangle. \quad (11)$$

The pair of “macroscopical” displacement  $u$  and the gradient Young measures  $\nu$  represents a quite natural *mesoscopical description* of the state of the body. The “kinematically” admissible pairs  $(u, \nu)$  are ultimately in the nonconvex set

$$Q := \left\{ (u, \nu) \in W^{1,p}(\Omega; \mathbb{R}^3) \times \mathcal{G}^p(\Omega; \mathbb{R}^{3 \times 3}); \int_{\mathbb{R}^{3 \times 3}} A \nu_x(dA) = \nabla u(x) \text{ for a.a. } x \right\}. \quad (12)$$

Within microstructure evolution due to time-varying loading  $F$ , the rate-independent dissipation again comes into play. Inspired by (6) with  $\mu_v = 0$ , we put

$$R(\nu) := \int_{\Omega} \delta_K^*(\lambda(x)) dx \quad \text{with} \quad \lambda(x) = \int_{\mathbb{R}^{3 \times 3}} \mathcal{L}(A) \nu_x(dA) dx. \quad (13)$$

The quantity  $\lambda$  plays the role of a macroscopical *volume fraction* assigned through (13) to the microstructure described by  $\nu$ .

Neglecting kinetic energy and based on *minimum-stored-energy principle* competing with *maximum-dissipation* (or rather *realizability* [17]) *principle*, makes a relevant base for microstructure evolution modelling provided a global *stability*

$$\forall t \geq 0, \forall (\tilde{u}, \tilde{\nu}) \in Q: \quad \bar{\Phi}(t, u(t), \nu(t)) \leq \bar{\Phi}(t, \tilde{u}, \tilde{\nu}) + R(\nu(t) - \tilde{\nu}) \quad (14)$$

can be accepted as relevant. Requiring still, for any  $0 \leq t_1 < t_2$ , the *energy equality*

$$\bar{\Phi}(t_2, u(t_2), \nu(t_2)) + \text{Var}_R(\nu; s, t) = \bar{\Phi}(t_1, u(t_2), \nu(t_2)) - \int_{t_1}^{t_2} \left\langle \frac{\partial F(t)}{\partial t}, u \right\rangle dt \quad (15)$$

where  $\text{Var}_R(\nu; t_1, t_2)$  denotes the total variation over  $[t_1, t_2]$  of  $\nu(\cdot)$  with respect to  $R$  from (13). Introduced in [18, 22, 23], (14)–(15) is a so-called *energetic formulation* of the relaxed problem.

Analysis of it in the context of SMA modelling is in [20] provided  $\bar{\Phi}$  is still regularized by counting energy of possible spatial variations in  $\lambda$ , as proposed in [9, p.364]. For computational implementation, additional discretization of the set  $Q$  is necessary. Canonical approach is to apply P1-finite elements on a triangulation of a polyhedral domain  $\Omega$  for discretization of  $u$  and element-wise constant (=homogeneous) so-called laminates (see [28]) to discretize  $\nu$ , see also [2, 15]. Computational simulation of experiments on NiMnGa and CuAlNi singlecrystals are in [16, 37].

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