

A NEW “FLEXIBLE” 3D MACROSCOPIC MODEL FOR SHAPE MEMORY ALLOYS

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ABSTRACT. In this paper we introduce a 3D phenomenological model for shape memory behavior, accounting for: martensite reorientation, asymmetric response of the material to tension/compression, different kinetics between forward and reverse phase transformation. We combine two modeling approaches using scalar and tensorial internal variables. Indeed, we use volume proportions of different configurations of the crystal lattice (austenite and two variants of martensite) as scalar internal variables and the preferred direction of stress-induced martensite as tensorial internal variable. Then, we derive evolution equations by a generalization of the principle of virtual powers, including microforces and micromovements responsible for phase transformations. In addition, we prescribe an evolution law for phase proportions ensuring different kinetics during forward and reverse transformation of the oriented martensite.

1. Introduction. In the last years shape memory alloys (SMAs) have been deeply investigated, from the point of view of modeling, analysis, and computation. Indeed, these materials present many important industrial applications (for example to aeronautical, biomedical, structural, and earthquake engineering) due to their characteristic of superelasticity and shape memory effect.

It is known that the shape memory effect is the consequence of a (reversible) martensitic phase transformation between different configurations of the crystal lattice in the alloy: from a high symmetric phase, austenite, to a lower symmetric configuration, martensite. Austenite is a solid phase (at high temperature) which can transform in martensite by means of a shearing mechanism. When transformation comes from thermal actions (lowering the temperature) the result is a multi-direction martensite, in which variants compensate each other and there is no resulting macroscopic deformation. On the contrary, when transformation is obtained by loading, oriented martensite is formed in the stress direction, exhibiting a macroscopic deformation.

In particular, the research have been developed towards the aim of finding a flexible phenomenological model. Some reliable models have been proposed to predict the response of such materials. Among the others, we focus on two models developed in the framework of phase transitions.

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The first, proposed by Frémond (cf., e.g., [7] and some generalizations [4], [5]), describes the behavior of shape memory in terms of (local) volume proportions of different configurations of the crystal lattice. More precisely, the austenite and two variants of martensite are taken into account. Note that the average behavior of different configurations is considered as the behavior of the equivalent single variant. The resulting model is able to describe phase transformation between different configurations. However, the model is obtained assuming that the direction of the transformation strain (associated to the detwinned martensite) is known.

The second model we are considering has been proposed in [10] and then studied in [2], and it assumes to deal with only one tensorial internal variable, i.e., the transformation strain tensor, which describes the direction of martensite. In addition, such a model leads to a simple and robust algorithm, based on a plasticity-like return map. Thanks to this property, the model has been used for implementation within finite element codes, allowing the simulation of complex SMA devices. However, some secondary effects are not included in this second model, as scalar and directional information are tightly interconnected.

Thus, one could wonder how to get a deeper description of micro-phenomena, possibly combining the main features of the two different approaches. Accordingly, the purpose of this paper is to combine the two cited theories, describing secondary effects in the phase transitions as well as directional information for the transformation strain. Thus, both scalar and tensorial internal variables are introduced, accounting for the phase proportions (assuming that in each point the phases may coexist with different proportions) and for the orientation of the transformation strain associated to the detwinned martensite. We consider both proportion and direction as internal variables and we write evolution equations for both of them. We recall that an attempt in this direction has been performed in [1] and in this respect the present model can be considered even as a further generalization, since we account for different kinetics during forward and reverse phase transformations. Moreover, we prescribe an evolution law to capture asymmetric response of the material in tension-compression loading. In [3] a 1D model has been introduced to describe this kind of phenomenon, using an asymmetric energy depending on a tensorial variable. However, it seems hard to extend such a model to higher dimensions. On the contrary, our approach (developing an asymmetric evolution theory for phase proportions) can apply to any space dimension.

As far as the analytical treatment of the model, this part is not developed in the present paper. However, let us point out that the resulting PDE system present interesting features also from the point of the proof of the existence (and uniqueness) of the solutions. Indeed, it combines strongly nonlinear equation with non-smooth constraint on the internal variables, quadratic nonlinearities and, in particular, a non-convex constraint on some tensorial variable.

2. The model. In this section we detail the derivation of the model. We mainly refer to the approach proposed by Frémond to describe the behavior of a thermo-mechanical system in terms of state and dissipative variables, as well as energy and dissipation functionals (see [7]). The main idea consists in assuming that (microscopic) phase transformations are due to micro-forces and micro-movements that have to be included in the global energy balance of the system (i.e. generalizing

the principle of virtual powers). In particular, the equations governing the evolution of internal variables are recovered as balance equations (as for the momentum balance).

2.1. The state and dissipative variables. As it is known, SMA phase transformations are due to transitions occurring in the microstructure configuration between austenite and twinned or detwinned martensite. In particular, detwinning manifests itself mainly through a shear strain so that we introduce a symmetric and deviatoric strain which appears in presence of the detwinned martensite. The (local) volume proportions of austenite and martensite variants is represented by phase parameters

$$\chi_A, \chi_M, \chi_S \in [0, 1], \quad \chi_A + \chi_M + \chi_S = 1. \tag{1}$$

More precisely, χ_A stands for austenite, χ_M for twinned martensite, and χ_S for detwinned martensite. Due to the internal constraint (1) on the phase proportions (coming from their physical meaning), we can restrict ourselves to consider just two independent phase variables (χ_M, χ_S) letting

$$\chi_A = 1 - \chi_M - \chi_S,$$

where

$$0 \leq \chi_M, \chi_S \leq 1, \quad \chi_M + \chi_S \leq 1.$$

Furthermore, \mathbf{d}^{tr} is the direction of the deviatoric strain tensor associated to the detwinned martensite with $\|\mathbf{d}^{tr}\| = \xi_s$ (ξ_s is the maximum amount for the detwinned martensite). Indeed, the deviatoric strain for detwinned martensite is given by $\chi_S \mathbf{d}^{tr}$. Then, θ is the absolute temperature, $\boldsymbol{\varepsilon}(\mathbf{u})$ the (symmetric) linearized strain tensor (\mathbf{u} is the vector of small displacements as we restrict ourselves to small deformations).

Finally, let us use the notation $\boldsymbol{\varepsilon}^e$ for the elastic component of the strain, so that it results

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \chi_S \mathbf{d}^{tr}.$$

Hence, the corresponding deviatoric strain \mathbf{e} is

$$\mathbf{e} := \boldsymbol{\varepsilon} - \frac{1}{3} \text{tr}(\boldsymbol{\varepsilon}) \mathbf{I}$$

\mathbf{I} being the identity matrix and $\text{tr}(\cdot)$ the trace operator. If $\boldsymbol{\sigma}$ is the Cauchy stress tensor, the deviatoric stress tensor \mathbf{S} is

$$\mathbf{S} := \boldsymbol{\sigma} - \frac{1}{3} \text{tr}(\boldsymbol{\sigma}) \mathbf{I} = \boldsymbol{\sigma} - \sigma_m \mathbf{I}.$$

As far as evolution, this is described by dissipative variables $\chi_{Mt}, \chi_{St}, \mathbf{d}_t^{tr}$, and $\nabla\theta$. These variables are in particular related to micro-velocities in the phase transformation.

Remark 1. Let us comment about the choice of state variables. The main idea consists in distinguishing between the norm and the direction of the inelastic strain. In this way, we are able to describe the presence of a product phase, to which a homogenized strain is associated, and a parent phase, in which it is active only the elastic strain. However, in the parent phase, we can also distinguish between the presence of twinned martensite and austenite. Thus, we get a more complex and, at the same time, more flexible description of the phenomenon with respect to the Souza and Frémond models (cf. [7], [10]).

2.2. The energy and dissipation functionals. We introduce the following free energy functional (depending on state variables) as a combination of the energies associated to the single variants (combined with suitable proportions) and by an interaction energy, accounting also for internal constraints

$$\Psi(\varepsilon, \mathbf{d}^{tr}, \chi_M, \chi_S, \theta) = \Psi_{el} + \Psi_{id} + \Psi_{ch} + \Psi_v \quad (2)$$

where

$$\Psi_{el} = \left(\frac{\lambda}{2} + \frac{\mu}{3} \right) (\text{tr } \varepsilon)^2 + \mu \|e - \chi_S \mathbf{d}^{tr}\|^2 \quad (3)$$

$$\Psi_{id} = c_s [(\theta - \theta_0) - \theta \log \theta]$$

$$\Psi_{ch} = (1 - \chi_M - \chi_S) h_A(\theta) + \chi_M h_M(\theta) + \chi_S h_S(\theta) + \mathbf{h}_d(\theta) : \mathbf{d}^{tr}$$

$$\Psi_v = I_K(\chi_M, \chi_S) + I_{\xi_s}(\|\mathbf{d}^{tr}\|) + \Psi_{int}(\chi_M, \chi_S).$$

Here $c_s > 0$ is the specific heat, $\theta_0 > 0$ a critical phase transition temperature, λ and μ are the Lamé constants; $h_A, h_S, h_M, \mathbf{h}_d$ are smooth thermal functions whose regularity will be specified later on (at least to ensure compatibility with thermodynamics). The function I_K is the indicator function of the convex set K

$$K := \{(\chi_M, \chi_S) \in \mathbf{R}^2 : 0 \leq \chi_M, \chi_S \leq 1, \chi_M + \chi_S \leq 1\},$$

i.e. it is $I_K(\chi_M, \chi_S) = 0$ if $(\chi_M, \chi_S) \in K$, while $I_K(\chi_M, \chi_S) = +\infty$ otherwise (cf. [7]). The function I_{ξ_s} forces $\|\mathbf{d}^{tr}\| = \xi_s$. Indeed, it is $I_{\xi_s}(\|\mathbf{d}^{tr}\|) = 0$ if $\|\mathbf{d}^{tr}\| = \xi_s$ and it is $+\infty$ otherwise. Ψ_{int} is a (sufficiently) smooth function accounting for interaction energy. As a possible choice for the interaction energy Ψ_{int} , we could simply consider

$$\begin{aligned} \Psi_{int}(\chi_M, \chi_S) &= C^{MS} \chi_M \chi_S + (C^{AM} \chi_M + C^{AS} \chi_S)(1 - \chi_M - \chi_S) \\ &\quad + C^{AMS} \chi_M \chi_S (1 - \chi_M - \chi_S), \end{aligned} \quad (4)$$

where $C^{MS}, C^{AM}, C^{AS}, C^{AMS}$ are positive constants.

Remark 2. The choice of the free energy is related to the models by Frémond and Souza, here extended to the novelty of our approach. In particular, let us comment about the choice of Ψ_{ch} in which thermal actions depend on thermal functions acting in the different configurations of the lattice (comparing with Souza's model in [10] the reader may refer to the term involving τ_M , and comparing with Frémond's model in [7] to the term related to the latent heat). The interaction energy Ψ_{int} can be seen as a sort of configurational energy associated with the coherency of the phases. It has been chosen in the form of a quadratic polynomial for the sake of simplicity. A similar choice can be found, e.g., in [5].

Remark 3. Note that for (χ_M, χ_S) we have introduced a convex constraint forcing $(\chi_M, \chi_S) \in K$. The constraint on \mathbf{d}^{tr} is convex w.r.t. to its norm as it is $\|\mathbf{d}^{tr}\| = \xi_s$, but not w.r.t. \mathbf{d}^{tr} . This point will represent a difficulty in solving the problem from the point of view of the existence of a solution (note that analogous difficulties arise in some liquid crystals models). For this reason, some suitable approximation of this constraint should be introduced to get the required existence result.

Now, let us introduce the pseudo-potential of dissipation, which is a positive convex functional depending on dissipative variables, vanishing for vanishing dissipation (cf. [9]). We have

$$\phi(\chi_{Mt}, \chi_{St}, \mathbf{d}_t^{tr}, \nabla \theta) = |\chi_{Mt}| + \phi_S(\chi_S, \boldsymbol{\sigma}, \chi_{St}) + \chi_S \|\mathbf{d}_t^{tr}\| + \frac{1}{2\theta} |\nabla \theta|^2. \quad (5)$$

Note that, ϕ is considered to possibly ensure an asymmetric behavior in tension and compression and for forward and backward transformation. This is due to the choice of the function ϕ_S (noting that it possibly depends on the stress and χ_S). Indeed, this choice generalizes the classical situation for rate-independent systems, where it is

$$\phi_S(\chi_S, \boldsymbol{\sigma}, \chi_{St}) = |\chi_{St}|. \tag{6}$$

Actually, ϕ_S is required to be rate independent with respect to χ_{St} . Hence, accounting for a possible dependence in the evolution on the stress (e.g., for tension-compression behavior) and on the volume of already detwinned martensite, we get as a further possible example

$$\phi_S(\chi_S, \boldsymbol{\sigma}, \chi_{St}) = d(\chi_S, \boldsymbol{\sigma})(\chi_{St})^+ + |\chi_{St}| \tag{7}$$

where $(f)^+ = f$ if $f \geq 0$ and $(f)^+ = 0$ if $f \leq 0$ and d is a sufficiently smooth function. From now on we deal in particular with (7).

Remark 4. Note that we could refine the model, e.g. adding in (7) a term as $\widehat{d}(\chi_S, \boldsymbol{\sigma})(\chi_{St})^-$ for decreasing evolution of the product phase.

2.3. The equations. We consider a smooth bounded domain $\Omega \subseteq \mathbf{R}^3$ with $\Gamma = \partial\Omega$ split into $\Gamma_1 \cup \Gamma_2$ (with Γ_i disjoint subset, Γ_1 with strictly positive measure).

We assume that a generalized version of the principle of virtual powers holds, accounting for internal microforces responsible for phase transitions (see [7]). Thus, the first principle of thermodynamics reads as follows

$$e_t + \operatorname{div} \mathbf{q} = r + \boldsymbol{\sigma} : \boldsymbol{\varepsilon}_t + B_M \chi_{Mt} + B_S \chi_{St} + \mathbf{B} : \mathbf{d}_t^{tr} \quad \text{in } \Omega, \tag{8}$$

the right hand side being the power of interior forces and the heat source r . Here, e is the internal energy, \mathbf{q} the heat flux, (B_M, B_S) and \mathbf{B} internal (microscopic) forces responsible for the phase transformation (i.e. the evolution of internal variables). The heat flux satisfies boundary condition (h is a known flux through the boundary)

$$\mathbf{q} \cdot \mathbf{n} = h \quad \text{on } \Gamma. \tag{9}$$

Hence, by the principle of virtual powers we get the quasi-static momentum balance

$$-\operatorname{div} \boldsymbol{\sigma} = \mathbf{f} \quad \text{in } \Omega, \tag{10}$$

with boundary condition

$$\mathbf{u} = \mathbf{0} \quad \text{on } \Gamma_1, \tag{11}$$

$$\boldsymbol{\sigma} \mathbf{n} = \mathbf{t} \quad \text{on } \Gamma_2, \tag{12}$$

\mathbf{f} being a volume force, while \mathbf{t} is a traction applied on a part of the boundary.

Analogously, the evolution of the phases depends on internal forces which are included in the energy balance of the system. Thus, we get two balance equations, one for the evolution of the phase proportions (related to (B_M, B_S)) and one for the evolution of the tensor \mathbf{d}^{tr} (related to \mathbf{B}), i.e.

$$(B_M, B_S) = (0, 0) \quad \text{in } \Omega, \tag{13}$$

$$\mathbf{B} = \mathbf{0} \quad \text{in } \Omega. \tag{14}$$

2.4. The constitutive relations. We need to prescribe constitutive relations for the involved physical quantities. The internal energy is

$$e = \Psi + \theta\eta$$

where the entropy η is prescribed by

$$\begin{aligned} \eta = -\frac{\partial\Psi}{\partial\theta} &= c_s \log \theta - h'_A(\theta)(1 - \chi_M - \chi_S) \\ &- h'_M(\theta)\chi_M - h'_S(\theta)\chi_S - \mathbf{h}'_d(\theta) : \mathbf{d}^{tr}. \end{aligned} \quad (15)$$

The Cauchy stress tensor is

$$\boldsymbol{\sigma} = \mathbf{S} + \sigma_m \mathbf{I},$$

with

$$\sigma_m = \frac{\partial\Psi}{\partial \operatorname{tr} \boldsymbol{\varepsilon}} = \left(\lambda + \frac{2}{3}\mu \right) \operatorname{tr} \boldsymbol{\varepsilon},$$

and

$$\mathbf{S} = \frac{\partial\Psi}{\partial \mathbf{e}} = 2\mu(\mathbf{e} - \chi_S \mathbf{d}^{tr}). \quad (16)$$

Hence, we get

$$(B_M, B_S) = (-B_M^{nd}, -B_S^{nd}) + (B_M^d, B_S^d) = \frac{\partial\Psi}{\partial(\chi_M, \chi_S)} + \frac{\partial\phi}{\partial(\chi_{Mt}, \chi_{St})}. \quad (17)$$

More precisely, letting

$$s(x) = \frac{x}{|x|} \text{ if } x \neq 0, \quad s(0) = [-1, 1],$$

and

$$H(x) = 1 \text{ if } x > 0, \quad H(x) = 0 \text{ if } x < 0, \quad H(0) = [0, 1]$$

there holds

$$\begin{aligned} B_M^{nd} &= h_A(\theta) - h_M(\theta) - \frac{\partial\Psi_{int}}{\partial\chi_M} - \gamma_M, \\ B_M^d &= s(\chi_{Mt}), \end{aligned} \quad (18)$$

and (choosing ϕ_S as in (7))

$$\begin{aligned} B_S^{nd} &= h_A(\theta) - h_S(\theta) - \frac{\partial\Psi_{int}}{\partial\chi_S} + 2\mu(\mathbf{e} - \chi_S \mathbf{d}^{tr}) : \mathbf{d}^{tr} - \gamma_S, \\ B_S^d &= \frac{\partial\phi_S}{\partial\chi_{St}} = s(\chi_{St}) + d(\chi_S, \boldsymbol{\sigma})H(\chi_{St}) \end{aligned} \quad (19)$$

with

$$(\gamma_M, \gamma_S) \in \partial I_K(\chi_M, \chi_S). \quad (20)$$

Finally, we consider

$$\mathbf{B} = -\mathbf{B}^{nd} + \mathbf{B}^d = \frac{\partial\Psi}{\partial \mathbf{d}^{tr}} + \frac{\partial\phi}{\partial \mathbf{d}_t^{tr}} \quad (21)$$

where

$$\begin{aligned} \mathbf{B}^{nd} &= 2\mu\chi_S(\mathbf{e} - \chi_S \mathbf{d}^{tr}) - \mathbf{h}_d(\theta) - \gamma \mathbf{d}^{tr} \\ \mathbf{B}^d &= \chi_S \mathbf{s}(\mathbf{d}_t^{tr}) \end{aligned} \quad (22)$$

using the notation

$$\mathbf{s}(\mathbf{d}_t^{tr}) = \frac{\mathbf{d}_t^{tr}}{\|\mathbf{d}_t^{tr}\|} \text{ if } \mathbf{d}_t^{tr} \neq 0, \quad \mathbf{s}(\mathbf{0}) = \{\mathbf{w} : \|\mathbf{w}\| \leq 1\}.$$

and letting

$$\gamma \in \frac{1}{\xi_s} \partial I_{\xi_s}(\|\mathbf{d}^{tr}\|) = \partial I_{\xi_s}(\|\mathbf{d}^{tr}\|).$$

Note that the constraint on $\|\mathbf{d}^{tr}\|$ is not convex w.r.t. to \mathbf{d}^{tr} , which represents a difficulty from a mathematical point of view (see Remark 3).

As far as the heat flux, we assume (Fourier law)

$$\mathbf{q} = -\theta \frac{\partial \Phi}{\partial \nabla \theta} = -\nabla \theta. \tag{23}$$

3. The PDE system.

3.1. The first principle. Combining constitutive relations with the balance laws, we get the PDE system we deal with. First let us discuss the energy balance, from which we show that the model is thermodynamically consistent. The equation governing the evolution of the temperature is recovered from (8). After using the chain rule and by the constitutive relations, we get

$$\theta(\eta_t + \operatorname{div} \frac{\mathbf{q}}{\theta}) - r = \frac{\partial \Phi}{\partial (\chi_{Mt}, \chi_{St})} \cdot (\chi_{Mt}, \chi_{St}) + \frac{\partial \Phi}{\partial \mathbf{d}_t^{tr}} : \mathbf{d}_t^{tr} + \frac{\partial \Phi}{\partial \nabla \theta} \cdot \nabla \theta \geq 0 \tag{24}$$

from which the second principle of thermodynamics follows, once $\theta > 0$ (it is the absolute temperature). Note in particular that we have strongly exploited the fact that $\partial \Phi$ turns out to be a maximal monotone operator with $\mathbf{0} \in \partial \Phi(\mathbf{0})$. The resulting equation is

$$\begin{aligned} &\theta_t(c_s - \theta(h''_M(\theta)\chi_M + h''_S(\theta)\chi_S + h''_A(\theta)(1 - \chi_M - \chi_S) + \mathbf{h}_d''(\theta) : \mathbf{d}^{tr})) \\ &+ \theta h'_A(\theta)(\chi_M + \chi_S)_t - \theta h'_M(\theta)\chi_{Mt} - \theta h'_S(\theta)\chi_{St} \\ &- \theta \mathbf{h}_d'(\theta) : \mathbf{d}_t^{tr} - \Delta \theta = |\chi_{Mt}| + |\chi_{St}| + d(\chi_S, \boldsymbol{\sigma})(\chi_{St})^+ + \chi_S \|\mathbf{d}_t^{tr}\| + r. \end{aligned} \tag{25}$$

In particular, we have to assume that $h_A, h_M, h_S, \mathbf{h}_d$ are smooth functions and

$$(c_s - \theta(h''_M(\theta)\chi_M + h''_S(\theta)\chi_S + h''_A(\theta)(1 - \chi_M - \chi_S) + \mathbf{h}_d''(\theta) : \mathbf{d}^{tr})) \geq C > 0.$$

Remark 5. This assumption is required to preserve parabolicity of the evolution equation (25). This assumption seems physically consistent and it is deeply used in the literature for this kind of problems (see [7]). Mainly, it is required that $h_A, h_M, h_S, \mathbf{h}_d$ are in $W^{2,\infty}$, and that their norms and $|h'_A(\xi)\xi| + |h'_M(\xi)\xi|$ is uniformly bounded by some sufficiently small constant (and the same for h_M, h_S, \mathbf{h}_d). This can be read as a smooth truncation of the standard choice for this kind of functions of type $L/\theta_*(\theta - \theta_*)$ (L being the latent heat and θ_* the phase transition temperature).

3.2. The evolution. Combining constitutive relations with momentum balance, it follows

$$-\operatorname{div} \left((\lambda + \frac{2}{3}\mu) \operatorname{tr} \boldsymbol{\varepsilon} \mathbf{I} + 2\mu(\mathbf{e} - \chi_S \mathbf{d}^{tr}) \right) = \mathbf{f}, \tag{26}$$

combined with (11), (12). Then, by definition of B_M and B_S , the evolution equations for (χ_{Mt}, χ_{St}) are written as

$$s(\chi_{Mt}) + (h_M(\theta) - h_A(\theta)) + \frac{\partial \Psi_{int}}{\partial \chi_M} + \gamma_M = 0 \tag{27}$$

and

$$\begin{aligned} s(\chi_{St}) + d(\chi_S, \boldsymbol{\sigma})H(\chi_{St}) + (h_S(\theta) - h_A(\theta)) - 2\mu(\mathbf{e} - \chi_S \mathbf{d}^{tr}) : \mathbf{d}^{tr} \\ + \frac{\partial \Psi_i n t}{\partial \chi_S} + \gamma_S = 0 \end{aligned} \quad (28)$$

where

$$(\gamma_M, \gamma_S) \in \partial I_K(\chi_M, \chi_S).$$

Note that $\partial I_K(\chi_M, \chi_S) = (0, 0)$ if (χ_M, χ_S) belongs to the interior of K , while it is given by the normal cone to the boundary if $(\chi_M, \chi_S) \in \partial K$.

Finally, the evolution equation for \mathbf{d}^{tr} is given by

$$\begin{aligned} \chi_S \mathbf{s}(\mathbf{d}_t^{tr}) - 2\mu \chi_S (\mathbf{e} - \chi_S \mathbf{d}^{tr}) + \mathbf{h}_d(\theta) + \gamma \mathbf{d}^{tr} = \mathbf{0}, \\ \gamma \in \partial I_{\xi_s}(\|\mathbf{d}^{tr}\|). \end{aligned} \quad (29)$$

Remark 6. Note that the coefficient χ_S of the evolution term $\mathbf{s}(\mathbf{d}_t^{tr})$ ensures that in the absence of detwinned martensite there is no dissipative contributions involving \mathbf{d}^{tr} .

3.3. An equivalent formulation. Let us now introduce (B_M and B_S are defined as in (18) and (19))

$$F_M(B_M^{nd}) = |B_M^{nd}| - R_M \quad (30)$$

$$F_S(B_S^{nd}) = |B_S^{nd}| - R(B_S^{nd}, \chi_S, \boldsymbol{\sigma}) \quad (31)$$

where

$$R(B_S^{nd}, \chi_S, \boldsymbol{\sigma}) = R_S \text{ if } B_S^{nd} < 0$$

$$\text{and } R(B_S^{nd}, \chi_S, \boldsymbol{\sigma}) = R_S + d(\chi_S, \boldsymbol{\sigma}) \text{ if } B_S^{nd} \geq 0.$$

Here the positive constant R_M, R_S are related to the coefficient of $s(\cdot)$ in the evolution equations for the phase parameters (in the previous paragraph it was $R_M = R_S = 1$) Then, we can rewrite the evolution of the phases (27) and (28) as follows

$$\chi_{Mt} = \zeta_M \frac{B_M^{nd}}{|B_M^{nd}|}, \quad (32)$$

$$\chi_{St} = \zeta_S \frac{B_S^{nd}}{|B_S^{nd}|}, \quad (33)$$

$$\zeta_i F_i = 0 \quad i = M, S, \quad (34)$$

$$F_i(B_i^{nd}) \leq 0, \quad i = M, S. \quad (35)$$

Note that F_i play the role of yield functions (see, e.g., [8]).

Analogously we may introduce

$$F_d = \|\mathbf{B}^{nd}\| - \chi_S$$

letting

$$\mathbf{d}_t^{tr} = \zeta_d \frac{\mathbf{B}^{nd}}{\|\mathbf{B}^{nd}\|},$$

with

$$\zeta_d F_d = 0, \quad F_d \leq 0.$$

4. **Some examples.** In the following we explore the model performances limiting the discussion only to the case of a proportional loading state, i.e., neglecting the reorientation process. Accordingly, to simplify the discussion, we set $\mathbf{h}_d(\theta) = \mathbf{0}$, \mathbf{d}^{tr} in the same direction of \mathbf{S} (and \mathbf{e}), assuming also $\mathbf{d}_t^{tr} = \mathbf{0}$. Under these simplifying positions, we may set (see (16))

$$\frac{\mathbf{B}^{nd}}{\|\mathbf{B}^{nd}\|} = \frac{\mathbf{e}}{\|\mathbf{e}\|} = \frac{\mathbf{d}^{tr}}{\|\mathbf{d}^{tr}\|}, \quad (36)$$

and

$$\|\mathbf{S}\| = 2\mu(\|\mathbf{e}\| - \chi_S). \quad (37)$$

Moreover, we distinguish between two different possible situations, one in which we consider only evolution of the stress-induced martensite and one in which we consider only evolution of the temperature-induced martensite, as discussed in the following. For both problems we start from a material completely in austenite (i.e., $\chi_S = \chi_M = 0$).

4.1. **Case 1: Temperature-induced effect.** For this problem we assume to start from $\boldsymbol{\sigma} = \mathbf{0}$ and to vary only the temperature. Accordingly, only a variation of χ_M can be produced.

The problem is governed by the following set of equations (see (18)):

$$\begin{cases} B_M^{nd} = h_A(\theta) - h_M(\theta) - \frac{\partial \Psi_{int}}{\partial \chi_M} - \gamma_M, \\ F_M(B_M^{nd}) = |B_M^{nd}| - 1 \\ \chi_{Mt} = \zeta_M \frac{B_M^{nd}}{|B_M^{nd}|}, \\ \zeta_M F_M = 0 \quad F_M(B_M^{nd}) \leq 0. \end{cases} \quad (38)$$

Here, we let $h_A(\theta) - h_M(\theta) = -C(\theta - \theta_0)$, θ_0 being a characteristic intrinsic temperature at which the two ideal phases are in equilibrium and C a material parameter. Then, let us take $R_M = 1$. We assume to first properly cool and then heat the material (see Figure 1).

In Figures 2-4 we report the evolution of the thermodynamic force B_M^{nd} versus the temperature θ , of the temperature-induced martensite χ_S versus the temperature θ , of the quantity γ_M versus the the temperature θ .

It can be observed that during cooling the model is able to reproduce a process in which the multi-variant martensite is produced and then during heating a process in which the multi-variant martensite is progressively extinguished. The forward and reverse phase transformations are perfectly symmetric.

4.2. **Case 2: Stress-induced effect.** For this problem we assume to start from $\boldsymbol{\sigma} = \mathbf{0}$ and to vary only the stress. Accordingly, only a variation of χ_S can be produced.

The problem is governed by the following set of equations ((19)):

$$\begin{cases} B_S^{nd} = h_A(\theta) - h_S(\theta) - \frac{\partial \Psi_{int}}{\partial \chi_S} + 2\mu(\|\mathbf{e}\| - \chi_S) - \gamma_S, \\ F_S(B_S^{nd}) = |B_S^{nd}| - R(B_S^{nd}, \chi_S, \boldsymbol{\sigma}) \\ \chi_{St} = \zeta_S \frac{B_S^{nd}}{|B_S^{nd}|}, \\ \zeta_S F_S = 0 \quad F_S(B_S^{nd}) \leq 0. \end{cases} \quad (39)$$

where (letting (7) holds)

$$\begin{aligned} R(B_S^{nd}, \chi_S, \boldsymbol{\sigma}) &= R_S \text{ if } B_S^{nd} < 0 \text{ and} \\ R(B_S^{nd}, \chi_S, \boldsymbol{\sigma}) &= R_S + d(\chi_S, \boldsymbol{\sigma}) \text{ if } B_S^{nd} \geq 0. \end{aligned} \quad (40)$$

Note that, once more we let $h_A(\theta) - h_M(\theta) = -C(\theta - \theta_0)$, θ_0 .

We assume to first properly load and then unload the material (see Figure 5).

In Figures 6-9 we report the evolution of the thermodynamic force B_S^{nd} versus the applied stress σ , of the stress-induced martensite χ_S versus the applied stress σ , of the quantity γ_S versus the applied stress σ , of the applied stress σ versus the strain ϵ .

Let us point out that the dependency of R_S from loading conditions is simplified indicating in the figures only $R_S(1)$ and $R_S(2)$, indicating the initial and final values associated with the forward phase transformation, and $R_S(3)$, indicating the initial and final values associated with the reverse phase transformation.

It can be observed that during loading the model is able to reproduce a process in which the single-variant martensite is produced and then during unloading a process in which the single-variant martensite is progressively extinguished. The forward and reverse phase transformation are unsymmetric.

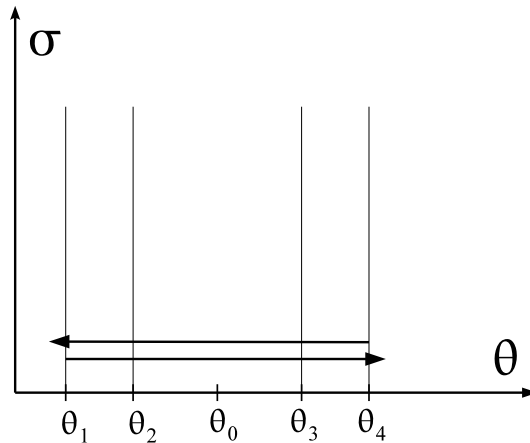


FIGURE 1. Temperature-induced test. Variation of the stress σ versus the temperature θ .

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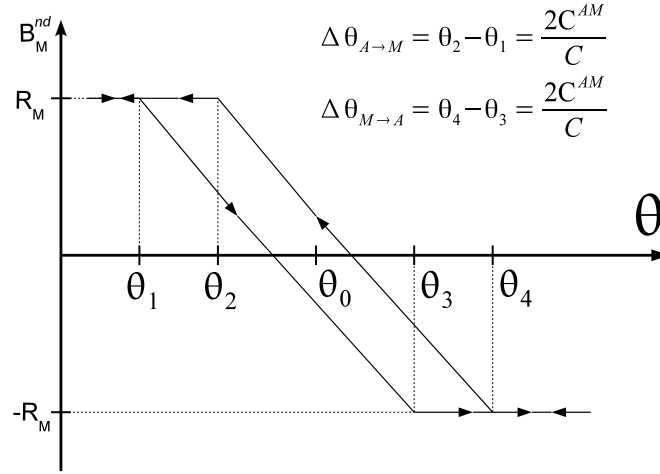


FIGURE 2. Temperature-induced test. Variation of the thermodynamic force B_M^{nd} versus the temperature θ .

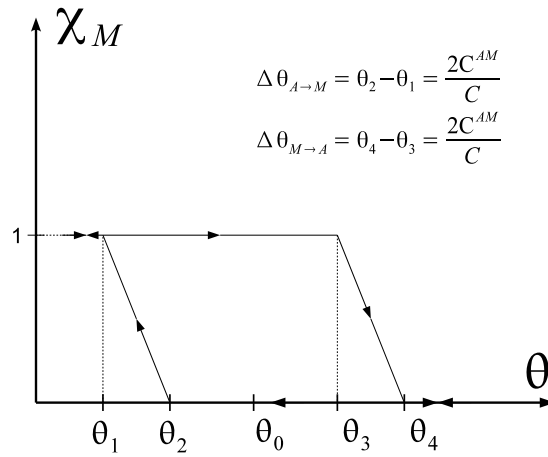


FIGURE 3. Temperature-induced test. Variation of the temperature-induced martensite χ_M versus the temperature θ .

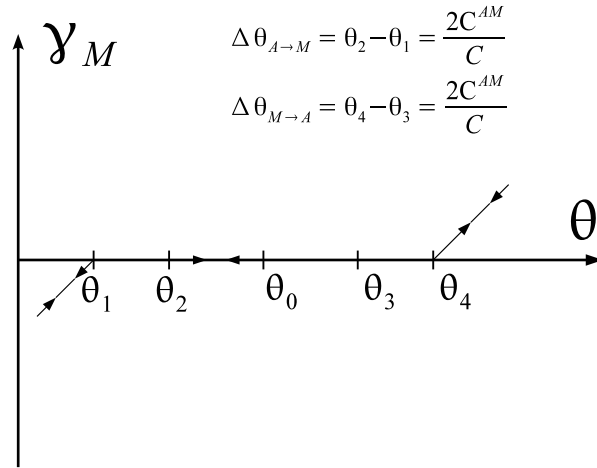


FIGURE 4. Temperature-induced test. Variation of the quantity γ_M versus the the temperature θ .

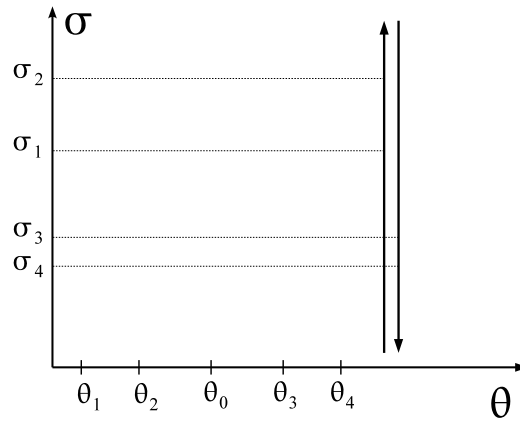


FIGURE 5. Stress-induced test. Variation of the stress σ versus the temperature θ .

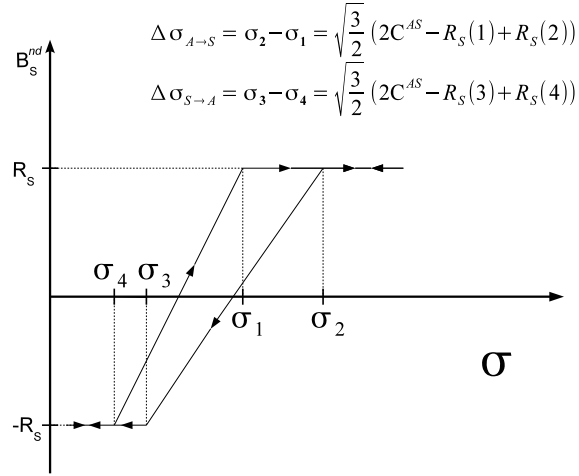


FIGURE 6. Stress-induced test. Variation of the thermodynamic force B_S^{nd} versus the applied stress σ .

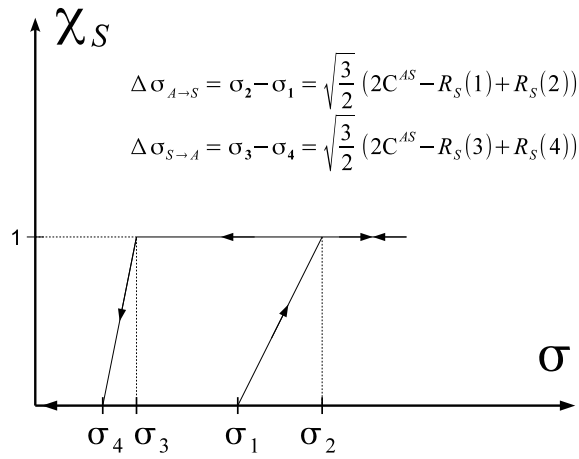


FIGURE 7. Stress-induced test. Variation of the stress-induced martensite χ_S versus the applied stress σ .

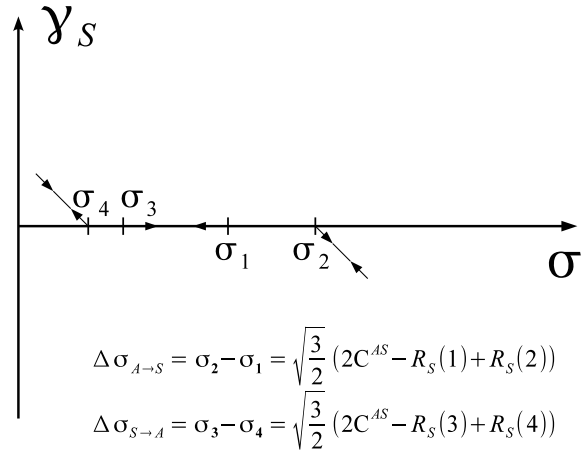


FIGURE 8. Stress-induced test. Variation of the quantity γ_S versus the applied stress σ .

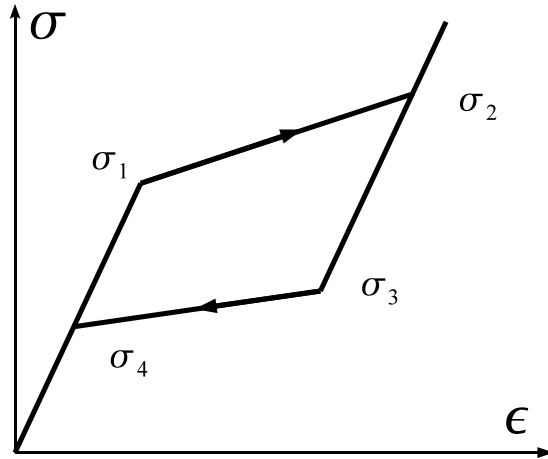


FIGURE 9. Stress-induced test. Variation of the applied stress σ versus the strain ϵ .

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