SMA structures computations

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Abstarct : Within the framework of the normal dissipative processes theory, a plasticity-like model is proposed for the shape memory alloys pseudoelastic behaviour. Its numerical implementation is performed using return mapping algorithms. Originally designed for elastoplasticity, this kind of algorithms requires suitable modifications in order to assure the uniqueness of the computed solution. A constitutive frame for proportional and non-proportional loading is also proposed for finite strains analysis.

Key-Words: SMA, Normal dissipative processes, Non-proportional loading, Finite strains

1 Introduction

The growing interest in smart structures technologies has led in the last decades to the formulation of a variety of constitutive models for shape memory alloys (SMA). However, most of these models are so demanding from a computational standpoint that, except some ones, their application has been limited to only one-dimensional situations.

In this work attention is focused on a phenomenological model of isotropic pseudoelasticity emanating from that originally presented in [1][2][3], and on its numerical integration. The constitutive model under consideration is formulated in the framework of internal variables theory of inelastic behaviours, namely, by defining the transition criteria determining the onset of phase transitions (SMA pseudoelasticity is a reversible behaviour associated with a stress-induced solid-solid phase transition from a parent phase called austenite to a product phase called martensite) in a way completely analogous to the loading functions of plasticity theory. Although consistent with classical rate-independent behaviour modelling, this approach requires, however, suitable modifications of numerical algorithms originally designed for elastoplasticity. Return mapping algorithms are discussed in detail hereafter.

In order to perform finite strains analysis, a closed form of the proposed modelling for small strains is developed within the context a non-material rotating frame formulation. In this context, a constitutive frame is suggested to take non-proportional loading into account.

2 Constitutive equations

From the thermodynamic point of view, the SMA pseudoelastic behaviour is irreversible. Nevertheless, a consistent modelling can be derived within the classical framework of the irreversible processes thermodynamics by using the concept of "constrained equilibrium" [4] according to which the rate of state variables or inelastic flows corresponding to some thermodynamic forces may vanish even though the forces are non-zero.

In order to derive the Helmholtz specific free energy function for SMA at "constrained equilibrium", the specific free energy of a solid two-phase mixture with interaction between the phases [1] can be used. Thus : $\psi = (1-z)\psi^a + z\psi^m + \psi^{di}$, z being the martensite volume fraction (the detwinned martensite variants are not distinguished), ψ^a and ψ^m the pure austenite and the pure martensite specific free energies respectively and ψ^{di} a specific coherency energy.

Assuming that both phases have equal mass density ρ and elastic stiffness matrix $\underline{\underline{E}}$, ψ^a and ψ^m can be chosen as : $\psi^a = \psi^a_{0R} + 1/2\rho^T \underline{\varepsilon}^a \underline{\underline{E}}\, \underline{\varepsilon}^a$ and $\psi^m = \psi^m_{0R} + 1/2\rho^T (\underline{\varepsilon}^m - \Delta\underline{\varepsilon})\, \underline{\underline{E}}\, (\underline{\varepsilon}^m - \Delta\underline{\varepsilon})$; $\underline{\varepsilon}^a$ and $\underline{\varepsilon}^m$ are the austenite and martensite intrinsic total strain tensors respectively and $\Delta\underline{\varepsilon}$ a strain tensor associated with the martensite creation.

$\psi^a_{0R} = u^a_{0R} - T_R\, s^a_{0R}$ and $\psi^m_{0R} = u^m_{0R} - T_R\, s^m_{0R}$ are the specific free energies of both phases at stress-free state and at a reference temperature T_R.

Considering that for a prescribed macroscopic total strain tensor $\underline{\varepsilon}$, $\underline{\varepsilon}^a$ and $\underline{\varepsilon}^m$ must comply with the Reuss bound model *i.e.* $\underline{\varepsilon} = (1-z)\,\underline{\varepsilon}^a + z\,\underline{\varepsilon}^m$, equilibrium conditions can be derived from the optimality conditions of the lagrangian function $\mathrm{L}_\psi = \psi + {}^T\left[\underline{\varepsilon} - (1-z)\,\underline{\varepsilon}^a - z\,\underline{\varepsilon}^m\right]\underline{\sigma}/\rho$ where $\underline{\sigma}$ is the macroscopic stress tensor [2]. At fixed z and $\underline{\varepsilon}$, it is shown that $\underline{\sigma}$ is equal to the stresses tensors in both phases *i.e.* $\underline{\sigma}^a = \rho\,\partial_{\varepsilon^a}\psi^a$ and $\underline{\sigma}^m = \rho\,\partial_{\varepsilon^m}\psi^m$. The Helmholtz specific free energy function of the two-phase system in "constrained equilibrium" can then be defined as a potential function for $\underline{\sigma} = \underline{\underline{E}}\,(\underline{\varepsilon} - \underline{\varepsilon}^{tr})$ where $\underline{\varepsilon}^{tr} = z\Delta\underline{\varepsilon}$ is the macroscopic inelastic strain tensor associated with the stress-induced phase transition. Thus:

$$\begin{aligned}\psi_{eq} &= \psi^a_{0R} - z\,\pi_{0R} \\ &\quad + \frac{1}{2\rho}\,{}^T(\underline{\varepsilon} - \underline{\varepsilon}^{tr})\,\underline{\underline{E}}\,(\underline{\varepsilon} - \underline{\varepsilon}^{tr}) + \psi^{di}; \qquad (1)\\ \pi_{0R} &= (u^a_{0R} - u^m_{0R}) - T_R\,(s^a_{0R} - s^m_{0R})\end{aligned}$$

The resulting intrinsic dissipation is:

$$\begin{aligned}\mathrm{D}^{mech} &= {}^T\underline{\sigma}\,\dot{\underline{\varepsilon}}^{tr} - R\,\dot{z} \geq 0; \\ R &= -\rho\,(\pi_{0R} - \partial_z\,\psi^{di})\end{aligned} \qquad (2)$$

The thermodynamic equilibrium states are those at which the intrinsic dissipation vanishes for any state admissible change. Depending on the form of the specific coherency energy ψ^{di}, these states define the turning points location for partial loading-unloading from "constrained equilibrium" states.

In absence of a good knowledge about the nucleation and growth of martensite within austenite leading to the exact form of ψ^{di}, the simplest function of $z(1-z)$ such as $\psi^{di} = 0$ for pure austenite $(z=0)$ and pure martensite $(z=1)$ has been proposed by Müller in [1], limiting the modelling to a behaviour type where the unstable equilibrium states are located along a single diagonal line.

In order to account for different configurations of unstable equilibrium states, a plasticity-like phenomenological approach can be used assuming two independent normal dissipative processes : one for the forward transition (austenite $\rightarrow$ martensite) characterised by $\dot{z} > 0$, the other for the reverse transition (martensite $\rightarrow$ austenite) characterised by $\dot{z} < 0$. Thus, D^{mech} is given at any time by two independent functions of $\dot{\underline{\varepsilon}}^{tr}$ and $\dot{z}$:

$$\begin{aligned}\mathrm{D}^{mech} &= \mathrm{D}_{am}\left\{(\dot{\underline{\varepsilon}}^{tr}, \dot{z}); (z; h_{am})\right\} \quad if \quad \dot{z} > 0 \\ \mathrm{D}^{mech} &= \mathrm{D}_{ma}\left\{(\dot{\underline{\varepsilon}}^{tr}, \dot{z}); (z; h_{ma})\right\} \quad if \quad \dot{z} < 0\end{aligned} \qquad (3)$$

h_{am} and h_{ma} are sets of history parameters [5] *i.e.* the energy dissipated during phase transitions is history dependent.

In the particular case of a rate-independent behaviour (plasticity-like behaviour), these functions are convex, positively homogeneous of degree one.

Since the forward transition (austenite $\rightarrow$ martensite) can be initiated in any loading direction, D_{am} is a quasi-positively homogeneous function defining a full convex cone in an eight-dimensions space such as $\mathrm{D}_{am}\left\{(\underline{0},0); (z; h_{am})\right\} = 0$. Following the generalised standard materials formalism, the phase transition kinetics $\dot{\underline{\varepsilon}}^{tr}$ and $\dot{z}$ belong to the subdifferential of the indicator function of the convex domain $\Omega_{am} = \left\{(\underline{\sigma}, R)\,/\,\varphi_{am}(\underline{\sigma}, R) \leq 0\right\}$ *i.e.* the elasto-dissipative domain. What leads to the maximum dissipation principle from which the normal evolution laws $\dot{\underline{\varepsilon}}^{tr} = \dot{\lambda}_{am}\,\partial_{\underline{\sigma}}\varphi_{am}$ and $\dot{z} = -\dot{\lambda}_{am}\,\partial_R\varphi_{am}$ are obtained. The Lagrange multiplier $\dot{\lambda}_{am}$ is derived from the consistency condition $\dot{\varphi}_{am} = 0$.

The normality of the phase transition rates direction to the yield surface φ_{am} has been clearly established experimentally in the case of a CuAlBe alloy [6] (Fig. 1).

Considering that the SMA behaviour is isochoric, asymmetric in tension-compression but symmetric in pure shearing, a formal equation of the yield surface φ_{am} could be [5]:

$$\begin{aligned}\varphi_{am} &= \Sigma(J_2, J_3) - \Sigma_{am}(z; h_{am}) \leq 0; \\ \Sigma_{am} &= \frac{1}{\gamma_{eq}}\left[R(z) + \Pi_{am}(z; h_{am})\right]\end{aligned} \qquad (4)$$

where Σ is an effective stress depending on the second (J_2) are and the third (J_3) invariant of the Cauchy stress tensor $\underline{\sigma}$, Σ_{am} the threshold stress in pure shearing and γ_{eq} the maximum phase transition strain in the equivalent stress-strain plane.

Thus:

$$\underline{\dot{\varepsilon}}^{tr} = \dot{\lambda}_{am}\, \partial_{\underline{\sigma}} \Sigma \qquad \dot{z} = \frac{\dot{\lambda}_{am}}{\gamma_{eq}} \qquad (5)$$

For a rate-independent and isotropic behaviour, Σ is a positively homogeneous function of degree one. Choosing $\Sigma = p\sqrt{3J_2}\,(1+q\,y_\sigma)^r$, where p, q and r are material parameters and $y_\sigma = 27\,J_3 / 2\,(3J_2)^{3/2}$, the tension-compression asymmetry is observed for different values of r, but for certain values of q a loss of convexity may occur. This problem can be avoided by using the alternative $\Sigma = \sqrt{3J_2}\; f(y_\sigma)$ where $f(y_\sigma) = \cos\left[\cos^{-1}\left[1 - a\,(1 - y_\sigma)\right]/3\right]$, $a \in [0,1]$ being material parameter [6].

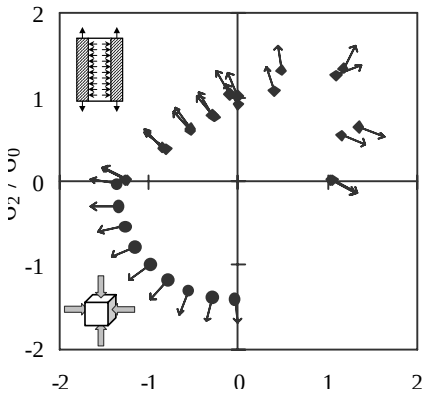

Fig.1: Forward phase transformation yield surface for a CuAlBe Alloy [6]

The definition of the threshold shear stress Σ_{am} needs the knowledge of the coherency energy ψ^{di} $(R(z) = ?)$ and the dissipation function D_{am} $(\Pi_{am}(z;h_{am}) = ?)$. In order to overcome these problems, a set of constitutive functions ("hardening functions" $f_{am}(z)$, turning points location functions $g_{am}(z)$) is used within the framework of a phenomenological approach (Fig. 2).

Since the inelastic strains must be recovered during the reverse transition (martensite $\rightarrow$ austenite), it comes from (5) that $D_{ma} = \Pi_{ma}(z;h_{ma})\,\dot{z}$ where $\Pi_{ma} < 0$ is the phase transition driving force. Proceeding like for the forward transition, one obtains then $\dot{z} = -\dot{\lambda}_{ma}\,\partial_{\Pi}\,\phi_{ma}$ with $\phi_{ma} = \Pi - \Pi_{ma}(z;h_{ma}) \geq 0$ and $\Pi = \gamma_{eq}{}^{T}\,\underline{\sigma}\,\partial_{\underline{\sigma}}\Sigma - R(z)$ [5]. The Lagrange multiplier $\dot{\lambda}_{ma}$ can be derived from the consistency condition $\dot{\phi}_{ma} = 0$ or $\dot{\varphi}_{ma} = 0$ with:

$$\varphi_{ma} = {}^{T}\underline{\sigma}\,\partial_{\underline{\sigma}}\Sigma - \Sigma_{ma}(z;h_{ma});$$
$$\Sigma_{ma} = \frac{1}{\gamma_{eq}}\left[R(z) + \Pi_{ma}(z;h_{ma})\right] \qquad (6)$$

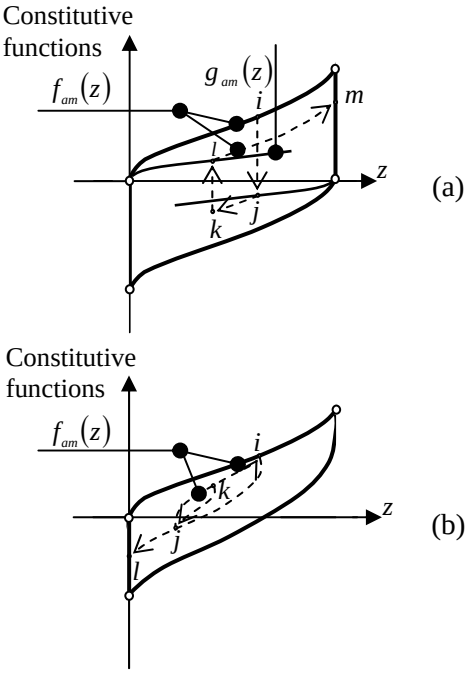

Fig. 2: Constitutive functions for phenomenological modelling in pseudoelasticity
(a) Internal loops with elastic domain
(b) Internal loops without elastic domain

But in both cases, it is necessary to know the inelastic strain rates $\dot{\underline{\varepsilon}}^{tr}$ as function of $\dot{z}$. What suggests a three-dimensional modelling which could be based, within the framework of a phenomenological approach, on a unique yield function φ_{ma} for all possible reverse transitions (contrary to the forward transition, the reverse transition can not occur in any direction). φ_{ma} delimits, in this case, a non-convex elastic domain when this domain exists (Fig. 3).

Following the classical plasticity formalism (generalised standard materials formalism), the use of the maximum dissipation principle in order to derive the complementary evolution laws requires a convex constrained region. Such a region can be

defined here by a function $\kappa(\underline{\sigma}, R; h_{ma}) = \kappa(\underline{\sigma}, z; h_{ma})$ such as:

$$\begin{aligned} &\kappa(\underline{\sigma}, z; h_{ma}) > 0 \text{ when } \Pi - \Pi_{ma}(z; h_{ma}) > 0 \\ &\kappa(\underline{\sigma}, z; h_{ma}) = 0 \text{ when } \Pi - \Pi_{ma}(z; h_{ma}) = 0 \end{aligned} \quad (7)$$

Choosing $\kappa(\underline{\sigma}, z; h_{ma}) = {}^{T}\underline{\sigma}\,\underline{D}_{\varepsilon^{tr}} - \Sigma_{ma}(z; h_{ma})$ where $\underline{D}_{\varepsilon^{tr}} = \underline{\varepsilon}^{tr} / \varepsilon_{eq}^{tr}$; $\varepsilon_{eq}^{tr} = \gamma_{eq} z$ (see also [3]) is the last inelastic strains direction before unloding, it comes then:

$$\begin{aligned} &\dot{\underline{\varepsilon}}^{tr} = -\dot{\lambda}_{ma}\, \partial_{\underline{\sigma}} \kappa = -\dot{\lambda}_{ma}\, \underline{D}_{\varepsilon^{tr}} \\ &\dot{z} = -\frac{\dot{\lambda}_{ma}}{\gamma_{eq}} \end{aligned} \quad (8)$$

Note that in the particular case of proportional loading, $\underline{D}_{\varepsilon^{tr}} = \partial_{\underline{\sigma}} \varphi_{am} = \partial_{\underline{\sigma}} \Sigma$ (Fig. 3).

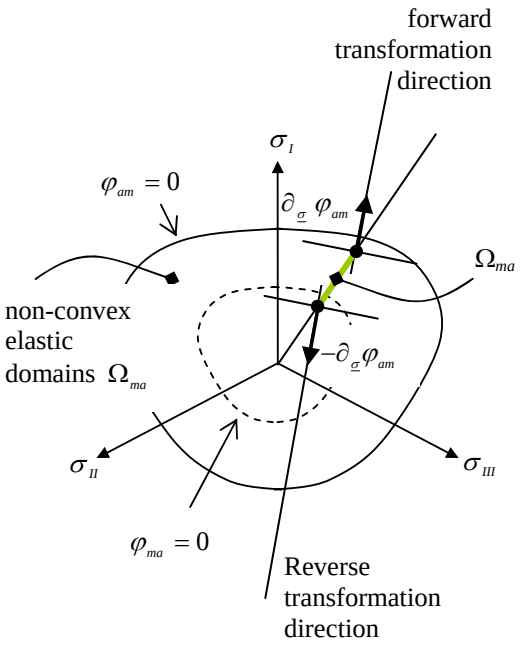

Fig. 3: Forward and reverse phase transitions yield surfaces

3 Discrete formulation

Within an incremental method associated with a Newton iterative scheme, the basic problem is to update the state of the material in a way consistent with the constitutive model knowing the total incremental strains $\Delta\underline{\varepsilon}$ over a time interval $[{}_{n}t, {}_{n+1}t]$. Hence, for the proposed modelling: $\{{}_{n}\underline{\sigma}, {}_{n}z\} + \Delta\underline{\varepsilon} \rightarrow \{{}_{n+1}\underline{\sigma}, {}_{n+1}z\}$, ${}_{n}(.)$ meaning the previous convergent quantities and ${}_{n+1}(.)$ the current ones. The relationships between these quantities are derived from the constitutive equations established in the previous section. Using a fully implicit integration scheme over the time interval $[{}_{n}t, {}_{n+1}t]$, it comes from the incremental stress-strain relationship $\dot{\underline{\sigma}} = \underline{\underline{E}}(\dot{\underline{\varepsilon}} - \dot{\underline{\varepsilon}}^{tr})$:

$$\begin{aligned} &{}_{n+1}\underline{\sigma} = {}_{n+1}\underline{\sigma}^{*} - \underline{\underline{E}}({}_{n+1}\underline{\varepsilon}^{tr} - {}_{n}\underline{\varepsilon}^{tr}); \\ &{}_{n+1}\underline{\sigma}^{*} = {}_{n}\underline{\sigma} + \underline{\underline{E}}\,\Delta\underline{\varepsilon} \end{aligned} \quad (9)$$

with, from the evolution laws (5) and (8):

$$\begin{aligned} {}_{n+1}\underline{\varepsilon}^{tr} - {}_{n}\underline{\varepsilon}^{tr} &= \Delta\lambda_{am}\, {}_{n+1}\left|\partial_{\underline{\sigma}}\Sigma\right. \\ &= \gamma_{eq}({}_{n+1}z - {}_{n}z)\, {}_{n+1}\left|\partial_{\underline{\sigma}}\Sigma\right. \end{aligned} \quad (10)$$

for the forward transition, and:

$$\begin{aligned} {}_{n+1}\underline{\varepsilon}^{tr} - {}_{n}\underline{\varepsilon}^{tr} &= -\Delta\lambda_{ma}\, \underline{D}_{\varepsilon^{tr}} \\ &= \gamma_{eq}({}_{n+1}z - {}_{n}z)\, \underline{D}_{\varepsilon^{tr}} \end{aligned} \quad (11)$$

for the reverse transition, ${}_{n+1}z$ verifying:

$$\begin{aligned} &\varphi_{am}({}_{n+1}\underline{\sigma}, {}_{n+1}z; h_{am}) = 0 \\ &\varphi_{ma}({}_{n+1}\underline{\sigma}, {}_{n+1}z; h_{ma}) = 0 \end{aligned} \quad (12)$$

Adopting a full Newton approach to solve the strain driven finite-step constitutive problem associated with the forward transition, one obtains at iteration *i+1*:

$$\begin{aligned} &\begin{bmatrix} \underline{\underline{G}} & \gamma_{eq}\, {}_{n+1}\left|\partial_{\underline{\sigma}}\Sigma\right. \\ {}^{T}\,{}_{n+1}\left|\partial_{\underline{\sigma}}\Sigma\right. & -{}_{n+1}\left|\partial_{z}\Sigma_{am}\right. \end{bmatrix}^{i} \begin{bmatrix} \delta_{n+1}\underline{\sigma}_{i}^{i+1} \\ \delta_{n+1}z_{i}^{i+1} \end{bmatrix} = \\ &\begin{bmatrix} -\underline{\underline{E}}^{-1}({}_{n+1}\underline{\sigma} - {}_{n+1}\underline{\sigma}^{*}) - \gamma_{eq}\,\Delta z\, {}_{n+1}\left|\partial_{\underline{\sigma}}\Sigma\right. \\ -\varphi_{am} \end{bmatrix}^{i} \end{aligned} \quad (13)$$

The 4-order tensor $\underline{\underline{G}} = \underline{\underline{E}}^{-1} + \gamma_{eq}\Delta z\, {}_{n+1}\left|\partial^{2}_{\underline{\sigma}\underline{\sigma}}\Sigma\right.$; $\Delta z = ({}_{n+1}z - {}_{n}z)$, being definite positive since it is the sum of the positive definite tensor $\underline{\underline{E}}^{-1}$ and of the positive semi-definite one (in the more general case) $\gamma_{eq}\Delta z\, {}_{n+1}\left|\partial^{2}_{\underline{\sigma}\underline{\sigma}}\Sigma\right.$ since φ_{am} is convex and $\gamma_{eq}\Delta z > 0$, this system can be reduced to compute ${}_{n+1}z$.

$$\delta_{n+1}z_i^{i+1} = \Big\{ {}_{n+1}^{T}\Big|\partial_{\underline{\sigma}}\Sigma\, \underline{\underline{G}}^{-1}\,[\underline{\underline{E}}^{-1}({}_{n+1}\underline{\sigma} - {}_{n+1}\underline{\sigma}^{*}) + \gamma_{eq}\,\Delta z_{n+1}\Big|\partial_{\underline{\sigma}}\Sigma] + \varphi_{am}\Big\} \Big/ \Big\{ {}_{n+1}\Big|\partial_z\Sigma_{am} + \gamma_{eq}\,{}_{n+1}^{T}\Big|\partial_{\underline{\sigma}}\Sigma\; \underline{\underline{G}}^{-1}\,{}_{n+1}\Big|\partial_{\underline{\sigma}}\Sigma\Big\}\Big|^{i} \qquad (14)$$

The building of a plasticity-like SMA pseudoelastic behaviour for the forward transiion, suggests the use of a classical predictor-corrector scheme to compute the material stress state (Table 1).

Elastic prediction : Compute a trial state for given total incremental strains $\Delta\underline{\varepsilon}$

$${}_{n+1}\underline{\sigma}^{*} = {}_{n}\underline{\sigma} + \underline{\underline{E}}\Delta\underline{\varepsilon}, \qquad {}_{n+1}z^{*} = {}_{n}z$$

Check the yield function $\varphi_{am}({}_{n+1}\underline{\sigma}^{*}, {}_{n+1}z^{*}; h_{am})$

$${}_{n+1}\underline{\sigma} = {}_{n+1}\underline{\sigma}^{*}, \qquad {}_{n+1}z = {}_{n+1}z^{*} \quad \text{if} \quad \varphi_{am} \le 0,$$

else

Inelastic correction : The final stress state is obtained as the closest-point projection of the trial stress state on the elastic domain. At iteration i+1

$${}_{n+1}z^{i+1} = {}_{n+1}z^{i} - \Big\{ {}_{n+1}^{T}\Big|\partial_{\underline{\sigma}}\Sigma\, \underline{\underline{G}}^{-1}\Big[\underline{\underline{E}}^{-1}({}_{n+1}\underline{\sigma} - {}_{n+1}\underline{\sigma}^{*}) + \gamma_{eq}\,\Delta z_{n+1}\Big|\partial_{\underline{\sigma}}\Sigma\Big] - \varphi_{am}\Big\} \Big/ \Big\{ {}_{n+1}\Big|\partial_z\Sigma_{am} + \gamma_{eq}\,{}_{n+1}^{T}\Big|\partial_{\underline{\sigma}}\Sigma\; \underline{\underline{G}}^{-1}\,{}_{n+1}\Big|\partial_{\underline{\sigma}}\Sigma\Big\}\Big|^{i}$$

$${}_{n+1}\underline{\sigma}^{i+1} = {}_{n+1}\underline{\sigma}^{i} - \Big[\underline{\underline{G}}^{i}\Big]^{-1}\Big[\underline{\underline{E}}^{-1}({}_{n+1}\underline{\sigma}^{i} - {}_{n+1}\underline{\sigma}^{*}) + \gamma_{eq}({}_{n+1}z^{i+1} - {}_{n}z)\,{}_{n+1}\Big|\partial_{\underline{\sigma}}\Sigma^{i}\Big]$$

Table1: Stress computation algorithm for the forward transition

The solution of the associated finite-step constitutive problem and the evaluation of the consistent tangent operator [7] require the inversion of the fourth-order tensor $\underline{\underline{G}}$. In this respect, it is proved in [8] that the assumption of isotropic behaviour entails an explicit representation formula for $\underline{\underline{G}}^{-1}$ as linear combination of dyadic and square tensor products. All tensor operations required to compute the coefficients of the adopted formula are carried out in intrinsic form.

For the reverse transition, since the elastic domain is not convex (Fig. 3), an intermediate correction step is necessary to assure the uniqueness of the computed solution (Table. 2). The intermediate correction step consists in the projection of the elastic trial stress state on the convex region defined by the dissipation potential function (7) (Fig. 4).

Elastic prediction : Compute a trial state for a given total incremental strains $\Delta\underline{\varepsilon}$

$${}_{n+1}\underline{\sigma}^{*} = {}_{n}\underline{\sigma} + \underline{\underline{E}}\Delta\underline{\varepsilon}, \qquad {}_{n+1}z^{*} = {}_{n}z$$

Check the yield function

$$\varphi_{ma}({}_{n+1}\underline{\sigma}^{*}; {}_{n+1}z^{*}, h_{ma})$$

$${}_{n+1}\underline{\sigma} = {}_{n+1}\underline{\sigma}^{*}, \qquad {}_{n+1}z = {}_{n+1}z^{*} \quad \text{if} \quad \varphi_{ma} \ge 0$$

(before going through the yield surface) else

Intermediate inelastic correction : Compute an intermediate inelastic state as the projection of the elastic trial stress state on the convex domain defined by

$$\kappa(\underline{\sigma}; {}_{n}z, h_{ma}) \ge 0$$

$${}_{n+1}z^{\kappa} = {}_{n}z + \frac{{}_{n+1}^{T}\underline{\sigma}^{*}\,\underline{D}_{\varepsilon^{tr}} - \Sigma_{ma}({}_{n}z, h_{ma})}{\gamma_{eq}\,{}^{T}\underline{D}_{\varepsilon^{tr}}\,\underline{\underline{E}}\,\underline{D}_{\varepsilon^{tr}}}$$

$${}_{n+1}\underline{\sigma}^{\kappa} = {}_{n+1}\underline{\sigma}^{*} - \gamma_{eq}({}_{n+1}z^{\kappa} - {}_{n}z)\,\underline{\underline{E}}\,\underline{D}_{\varepsilon^{tr}}$$

Inelastic correction :

The final stress state is obtained as the closest-point projection of the intermediate inelastic stress state on the internal boundary of the elastic domain. Enforcing the yield condition

$$\varphi_{ma}({}_{n+1}\underline{\sigma}, {}_{n+1}z; h_{ma}) = \varphi_{ma}({}_{n+1}z; h_{ma}) = 0,$$

it comes at iteration i+1

$${}_{n+1}z^{i+1} = {}_{n+1}z^{i} + \frac{\varphi_{ma}({}_{n+1}z^{i}; h_{ma})}{\gamma_{eq}\,{}_{n+1}^{i}\Big|\partial_{\underline{\sigma}}\Sigma^{i}\,\underline{\underline{E}}\,\underline{D}_{\varepsilon^{tr}} + {}_{n+1}\Big|\partial_z\Sigma^{i}_{ma}}$$

$${}_{n+1}\underline{\sigma} = {}_{n+1}\underline{\sigma}^{\kappa} - \gamma_{\Sigma}({}_{n+1}z - {}_{n+1}z^{\kappa})\,\underline{\underline{E}}\,\underline{D}_{\varepsilon^{tr}}$$

Table 2: Stress computation algorithm for the reverse transition

4 Finite strains modelling

The approach used to build a finite transformations kinematics for the SMA themomechanical behaviour study is based on the concept of deformed intermediate configuration introduced for the first time by Eckart [10] and the notion of director vectors due to Cosserat and Cosserat [11], resumed by Mandel [12].

In the case of the SMA, the director vectors notion allows to orient and then to fix a non-relaxed intermediate configuration associated to the phase transition in the material. Assuming an elastic behaviour independent of the state phase, the

following decomposition of the transformation gradient is introduced:

$$\underline{F} = (\underline{I} + \underline{\varepsilon}^{e})\, q\, \underline{F}^{in} \qquad (15)$$

$\underline{F}^{in}$ is the transformation gradient due to phase transition and re orientation allowing to connect a reference configuration to an intermediate one in which a director frame linked somehow to the material internal structure preserves its initial orientation. The evolution of this frame up to the current configuration, in which the elastic deformations $\underline{\varepsilon}^{e}$ ($\|\underline{\varepsilon}^{e}\| << 1$) are measured, is defined by the rotation q ($\underline{q}^{T}\underline{q} = \underline{I}$; $\det \underline{q} = 1$).

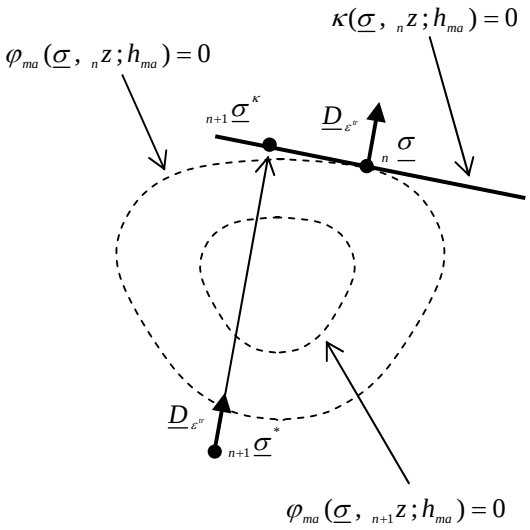

Fig. 4: Intermediate step for the stress computation in the reverse transformation

The SMA are characterized by a possible reversible phase transition austenite ↔ martensite. Their behaviour being associated with solid-solid phase transition according to specific planes called habit planes, an orthonormal direct frame defined by these planes as an average of their orientation can be considered as director (Fig. 5).
The expression of the total deformation gradient (15) leads to the following decomposition of the material strain rate tensor $\underline{D} = \left[\dot{\underline{F}}\underline{F}^{-1}\right]^{S}$ in the intermediate configuration ($(\underline{.})_{q} = {}^{T}\underline{q}\,(\underline{.})\,\underline{q}$):

$$\dot{\underline{d}}_{q} = \dot{\underline{\varepsilon}}^{e}_{q} + \dot{\underline{d}}^{in}_{q}; \qquad \dot{\underline{d}}^{in}_{q} = \left[\dot{\underline{F}}^{in}\,\underline{F}^{in-1}\right]^{S} \qquad (16)$$

$\underline{d}_{q}$ is a cumulated tensorial deformation in the sense introduced by Gilormini *et al.* [13].

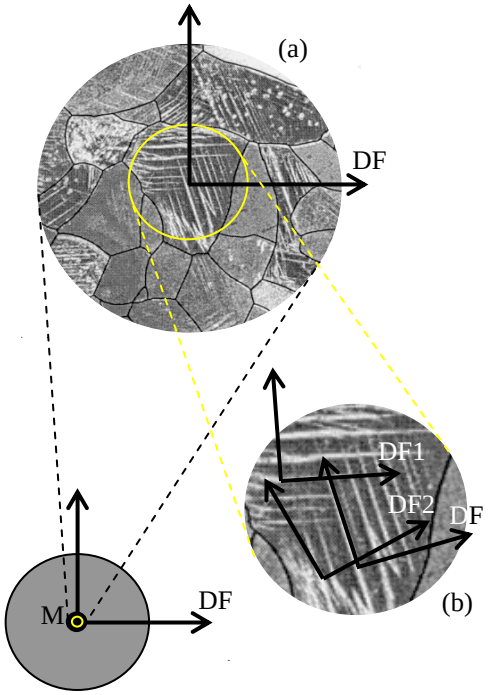

Fig. 5: (a) RVE Director Frame
(b) Director Frame linked to the habit planes

The intermediate configuration can be defined through the decomposition of the material spin $\underline{W} = \left[\dot{\underline{F}}\underline{F}^{-1}\right]^{A}$ in the current configuration, by solving:

$$\dot{\underline{q}} = (\underline{W} - \underline{W}^{tr}); \qquad \underline{q}\big|_{t=0} = \underline{I};$$
$$\underline{W}^{tr} = \underline{q}\left[\dot{\underline{F}}^{in}\,\underline{F}^{in-1}\right]^{A}\,{}^{T}\underline{q} \qquad (17)$$

That is why the knowledge of the spin $\underline{W}^{in}$ of the material milieu, as regards its material structure, is needed. Beyond the micro-macro approach seeming to be more natural to get this knowledge, the use of anti-symmetric isotropic tensorial functions representation theorems or the choice of a kinematics rotation consistent toward a phenomenological approach, are both other possibilities to assess the value of $\underline{W}^{in}$. For random or pseudo-random distributions of the habit planes, a family of objective kinematics rotations $\underline{q}$ can be defined by solving the following differential problem:

$$\dot{\underline{q}} = \left[(1-\alpha)\underline{W} + \alpha \dot{\underline{R}}^{T}\underline{R}\right]\underline{q}; \qquad \underline{q}\Big|_{t=0} = \underline{I}; \qquad \alpha \in]0,1] \tag{18}$$

where $\underline{R}$ is the proper rotation associated with $\underline{F}$.

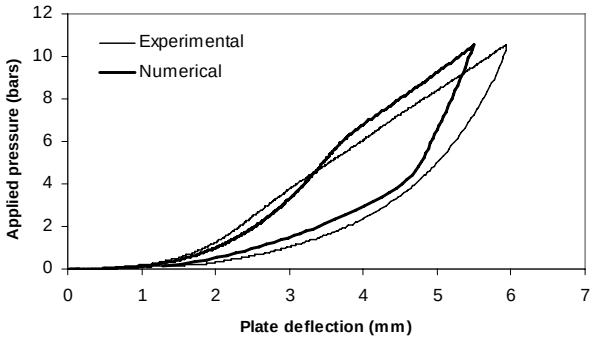

Fig. 6 : Bulging test on a CuAlBe plate [7] (thickness = 100 μm)

5 Non-proportionnal loading

Assuming that the state of the material in the intermediate configuration is completely decribed localy by the cumulated tensoral strains $\underline{d}_q$ and the inelastic strains $\underline{d}_q^{in} = \int_t \dot{\underline{d}}_q^{in} dt$ which consist on one part due to phase transition and another one due to re orientation, a tensorial hardening variable $\underline{\alpha}$, a scalar hardening variable α, the volume fraction of martensite *z* and the temperature *T*, the Clausius-Duhem inequality gives the following state law in the case of homogeneous and isothermal loading:

$$\underline{\sigma}_q = \rho \frac{\partial \psi}{\partial \underline{d}_q}; \quad \underline{\sigma}_q = {}^{T}\underline{q}\,\underline{\sigma}\,\underline{q} \tag{19}$$

and the intrinsic dissipation:

$$\mathrm{D}^{mech} = {}^{T}\underline{\dot{d}}_q^{in}\,\underline{\sigma}_q - {}^{T}\underline{\dot{\alpha}}\,\underline{X} - \dot{\alpha} X - \dot{z} R \geq 0 \tag{20}$$

with $\underline{X} = \rho\,\partial\psi/\partial\underline{\alpha}$, $X = \rho\,\partial\psi/\partial\alpha$, and $R = \rho\,\partial\psi/\partial z$, ψ being the specific free energy function:

$$\psi = \psi\left\{\underline{d}_q, \underline{d}_q^{in}, \underline{\alpha}, \alpha, z, T\right\} = \psi\left\{\underbrace{(\underline{d}_q - \underline{d}_q^{in})}_{\underline{\varepsilon}_q^e}, \underline{\alpha}, \alpha, z, T\right\} \tag{21}$$

Its expression can be given as a polynomial of the integrity basis terms associated to the second order symmetric tensors $\underline{\varepsilon}_q^e$ and $\underline{\alpha}$ for the complete orthogonal group:

$$\begin{aligned}\rho\psi &= \psi_{0R}^{a} - z\,\pi_{0R} \\ &+ \frac{1}{2}\lambda\left(tr\,\underline{\varepsilon}_q^e\right)^2 + \mu\, tr\left(\underline{\varepsilon}_q^e\right)^2 \\ &+ \left[\lambda\left(tr\,\underline{\varepsilon}_q^e\right)\left(tr\,\underline{\alpha}\right) + \mu\, tr\left(\underline{\varepsilon}_q^e\,\underline{\alpha}\right)\right]H_{NP} \\ &+ \delta\, tr\,\underline{\alpha}^2 + f(\alpha) + \psi^{di}(z,T)\end{aligned} \tag{22}$$

λ and μ are the Lamé coefficients, δ a positive material parameter, *f* a convex function of α and the Heaviside function H_{NP} ($H_{NP}=1$ for proportional loading, $H_{NP}=0$ for non-proportional loading). The term $\left[\lambda\left(tr\,\underline{\varepsilon}_q^e\right)\left(tr\,\underline{\alpha}\right) + \mu\, tr\left(\underline{\varepsilon}_q^e\,\underline{\alpha}\right)\right]H_{NP}$ is the expression of a neutral coupling between pure creation and re orientation of martensite. It allows us to preserve an inactive centred to the origin re orientation yield function for any proportional loading in the stress space (Fig.7).

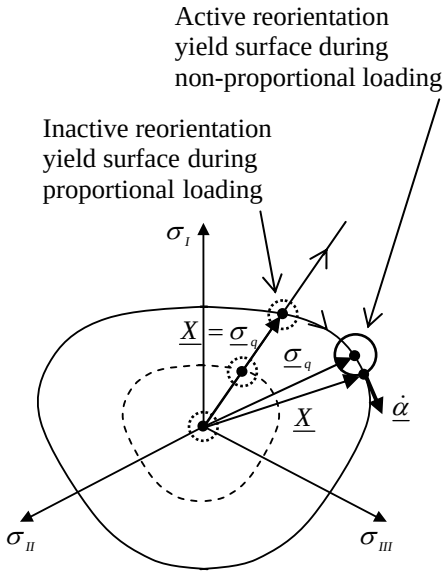

Fig. 7: Re orientation yield surface during non-proportional loading

Assuming that the phase transition or martensite creation (index *tr*) and re orientation (index *re*) phenomena remain uncoupled, the following evolution laws can be established considering rate independent normal dissipative processes:

$$\begin{aligned}
\underline{\dot{d}}^{in} &= \dot{\lambda}_{tr}\frac{\partial\varphi_{tr}\left(\underline{\sigma}_q,R\right)}{\partial\underline{\sigma}_q}+\dot{\lambda}_{re}\frac{\partial\varphi_{re}\left(\underline{\sigma}_q,\underline{X},X\right)}{\partial\underline{\sigma}_q}\\
\dot{z} &= -\dot{\lambda}_{tr}\frac{\partial\varphi_{tr}\left(\underline{\sigma}_q,R\right)}{\partial R}\\
\underline{\dot{\alpha}} &= -\dot{\lambda}_{re}\frac{\partial\varphi_{re}\left(\underline{\sigma}_q,\underline{X},X\right)}{\partial\underline{X}}\\
\dot{\alpha} &= -\dot{\lambda}_{re}\frac{\partial\varphi_{re}\left(\underline{\sigma}_q,\underline{X},X\right)}{\partial X}\\
\underline{\dot{X}} &= \underline{\dot{\sigma}}_q H_{NP}+\delta\underline{\dot{\alpha}}
\end{aligned} \qquad (23)$$

In the case of pure creation, the constitutive frame built in the hypothesis of small strains can be extended for finite strains analysis by using the corresponding quantities in the intermediate configuration. For forward transformations $\dot{\lambda}_{tr}=\dot{\lambda}_{am}$, $\varphi_{tr}=\varphi_{am}\left(\underline{\sigma}_q,R;h_{am}\right)$ and for reverse ones $\dot{\lambda}_{tr}=-\dot{\lambda}_{ma}$, $\varphi_{tr}=\kappa\left(\underline{\sigma}_q,R;h_{ma}\right)={}^{T}\underline{d}_q^{tr}\underline{\sigma}_q/(d_q^{tr})_{eq}-\Sigma_{ma}$ Numerical integration in a shell context and applications are presented in [7]. See also [14] for the computation of a consistent tangent operator.

6. Conclusion

A systematic approach for modelling of the SMA pseudoelasticity is proposed in this paper which correct and extend a previous one [15]. Based on the hypothesis of two independent normal dissipative processes : one for the formaward transition (austenite $\rightarrow$ martensite), the other for the reverse one (martensite $\rightarrow$ austenite), this approach leads to a plasticity-like class of models. Their numerical integration using algorithms originally designed for elastoplasticity, requires suitable modifications in order to insure the uniqueness of the computed solutions. An extension of this modelling has been performed for finite strains analysis using a non-material rotating frame formulation. The performances of such an approach have been tested in a specific shell context for thin structures analysis through a set of experiment [7]. The test of the proposed modelling in the case of non-proportional loading is in progress. The director frame updating in the case of oriented sub-structure remains an open problem.

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References

1. Y. Huo, I. Müller, Nonequilibrium thermodynamics of pseudoelasticity, *Continuum Mech. Thermodyn.*, 5, 1993, pp.163-204.
2. B. Raniecki, Ch. Lexcellent, K. Tanaka, Thermodynamic models of pseudoelastic behaviour of shape memory alloys, *Arch. Mech.*, 44, 1992, pp. 261-284.
3. J. G. Boyd, D. C. Lagoudas, A thermodynamical constitutive model for shape memory materials. Part I : the monolithic shape memory alloy", *Int. J. of Plasticity*, Vol. 12, n° 6, 1996, pp. 805-842.
4. R. J. Rice, Inelastic constitutive relations for solids : an internal variable theory and its application to metal plasticity, *J. Mech. Phy. Solids*, 19, 1971, pp. 433-455.
5. M. L. Boubakar, *De la modélisation théorique ou numérique de matériaux composites ou à transition de phase*, HDR Thesis of Franche-Comté University, France, n° 111, 2002.
6. Ch. Bouvet, *De l'uniaxial au multiaxial : comportement pseudoélastique des alliages à mémoire de forme*, PhD Thesis of Franche-Comté University, France, 2001.
7. B. Vieille, *Modélisation phénoménologique et intégration numérique du comportement superélastique des alliages à mémoire de forme en transformations finies*, PhD Thesis of Franche-Comté University, France, 2003.
8. V. Palazzo, L. Rosati, N. Valoroso, Solution procedures for J_3 plasticity and viscoplasticity, *Comput. Methods Appl. Mech. Engrg.*, 191, 2001, pp. 903-939.
9. B. Vieille, M. L. Boubakar, Ch. Lexcellent, Non-associated superelasticity in rotating frame formulation, *J. Theoretical Appl. Mech.*, 41, 3, 2003, pp. 675-691.
10. C. Eckart, The thermodynamics of irreversible processes: IV. The theory of elasticity and anelasticity, *Physical Review*, 72, pp. 373, 1948.
11. E. Cosserat, F. Cosserat, *Théorie des corps déformables*, Hermann, Paris, 1909.
12. J. Mandel, *Plasticité et viscoplasticité*, Cours CISM 97, Udine-Springer, New-York, 1971.
13. Gilormini, P. Roudier, P. Rougée, Les déformations tensorielles cumulées, *Study of the Académie des Sciences*, 316, Série 2, 1993, pp. 1499-1504.
14. M. L. Boubakar, B. Vieille, P. Boisse, Superelastic shell structures modelling. Part1 : Element formulation, *Comput. Methods Appl. Mech. Engrg.*, 194, 50-52, 2005, pp. 5273-5294.

15. M.L. Boubakar, N. Valoroso, B. Vieille, Remarks on the implementation of a class of isotropic pseudoelastic models for shape memory alloys, 6th Cansmart Workshop on Smart Materials and Structures, Montréal, Québec, Canada, 2003.

Appendix: Hardening functions for a strong history dependent pseudoelastic behaviour

Considering the behaviour depcited fig. 2.b, the bounding loop hardening function $f_{am}(z) = \sigma^{\Delta} f(z)$ is introduced for the forward transition, with:

$$f(z) = (1 - n/4)\, z + n[(z - 1/2)^3 + 1/8] \qquad (24)$$

σ^{Δ} and $n \in [0,4]$ are material parameters [6].

If we unload at point *i*, the corresponding martensite volume fraction z_i^M is memorised *i.e.* $h_{ma} = \{z_i^M\}$. For the reverse transition between points *i* and *j*, the hardening function is:

$$f_{ma}(z) = f_{ma}^{i} + f(z / z_i^M)[f_{am}(z_i^M) - f_{ma}^{i}] \qquad (25)$$

with $f_{ma}^{i} = -\hat{\sigma}^{\Delta} z_i^M$; $\hat{\sigma}^{\Delta}$ is a material parameter.

If we reload at point *j*, the corresponding martensite volume fraction z_j^m is memorised with z_i^M *i.e.* $h_{am} = \{z_i^M, z_j^m\}$. Between *j* and *l*, the hardening function is:

$$\begin{aligned} f_{am}(z) &= f_{ma}(z_j^m) \\ &+ f[(z - z_j^m)/(z_i^M - z_j^m)] \\ &\quad [f_{am}(z_i^M) - f_{ma}(z_j^m)] \end{aligned} \qquad (26)$$

If we hand the point *l* and reload up to *i*, the internal loop (*iji*) is closed and the history parameters z_i^M and z_j^m are then cancelled *i.e.* $h_{am} = h_{ma} = \{\phi\}$. Beyond *i* the phase transformation is driven by $f_{am}(z) = \sigma^{\Delta} f(z)$.

Nevertheless, if we unload at point *l*, the corresponding martensite volume fraction z_l^M is memorised *i.e.* $h_{am} = \{z_i^M, z_j^m, z_l^M\}$ and the hardening function is:

$$\begin{aligned} f_{ma}(z) &= f_{am}(z_l^M) \\ &+ f[(z_l^M - z)/(z_l^M - z_j^m)] \\ &\quad [f_{ma}(z_j^m) - f_{am}(z_l^M)] \end{aligned} \qquad (27)$$

Following this scheme, the hardening functions form can be easily generalised by recurrence.