ON THE CONSTITUTIVE MODELING AND NUMERICAL IMPLEMENTATION OF SHAPE MEMORY ALLOYS UNDER MULTIAXIAL LOADINGS - PART I: CONSTITUTIVE MODEL DEVELOPMENT AT SMALL AND FINITE STRAINS




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ABSTRACT

In this two-part paper, we review different aspects of shape memory alloys (SMAs), i.e., experimental observations, constitutive model development, numerical implementation and finite deformation effects.

In Part I, we present a short review on different mechanical behaviors of SMAs and classify them into primary and secondary effects which somehow shows the degree of importance of each behavior in different applications. We then present different approaches in constitutive modeling and highlight the phenomenological ones based on continuum thermodynamics with internal variables. Afterward, we propose a general structure of a SMA constitutive model in the small strain regime able to capture only primary effects. Moreover, we mention some recently proposed constitutive models and compare them from different aspects. We show that the proposed constitutive model has a general form and includes several constitutive models available in the literature.

We then extend a small-strain constitutive model into a finite strain regime. We specifically consider the approaches based on the multiplicative decomposition of the deformation gradient into elastic and transformation parts and review the so far proposed constitutive models available in the literature. We investigate some improvements for finite strain constitutive models from theoretical point of view.

As an important part of this study, we present the numerical counterpart in Part II.

1. MECHANICAL BEHAVIOUR OF SMAs

Intelligent, smart or functional materials exhibit special properties that make them a suitable choice for industrial applications in many branches of engineering. Among different types of smart materials, shape memory alloys (SMAs) have unique features known as pseudo-elasticity or super-elasticity, one-way and two-way shape memory effects [1,2]. Nowadays pseudo-elastic Nitinol is a common and well-known engineering material in the medical industry [2].

The origin of SMA material features is a reversible thermo-elastic martensitic phase transformation between a high symmetry, austenitic phase and a low symmetry, martensitic phase. Austenite is a solid phase, usually characterized by a body-centered cubic crystallographic structure, which transforms into martensite by means of a lattice shearing mechanism. When the transformation is driven by a temperature lowering, martensite variants compensate each other, resulting in no macroscopic deformation. However, when the transformation is driven by the application of a load, specific martensite variants favorable to the applied stress direction are preferentially formed, exhibiting a macroscopic shape change in the direction of the applied stress. Upon unloading or heating, this shape change disappears through the reversible conversion of the martensite variants into the parent phase [1].

Pseudo-elasticity and shape memory effect can be considered as primary effects and a SMA constitutive model have to capture these phenomena. We then can call other SMA mechanical behaviors as secondary effects which include:

- differences between the SMA response in tension and compression
- differences between the elastic properties at different phase transformation levels
- thermo-mechanical coupling effects
- residual inelastic strain effects
- subloops and return point memory effects

We call *basic* a constitutive model if it is capable to capture only primary effects without secondary ones. However, in some applications also secondary effects could be of interest. For example, in SMA actuators, residual inelastic strain can be important. It is then crucial to extend the basic model in order to take into account these secondary but important effects. It is possible to find some approaches in the literature which include the secondary effects in a basic constitutive model, see, i.e., [3-11]. Following this categorization is very useful since we first develop a successful basic constitutive model and then we add other (needed) secondary effects to the basic one. It also shows the importance of developing a successful basic model. To this end, in the next section we present a basic constitutive model which seems to be successful in capturing properly the primary effects.

We now consider another important aspect of SMA behaviour which is related to the primary effects. Several experimental studies show that the so-called variant reorientation can be assumed as the main phenomenon in non-proportional loadings of SMAs [12-16]. Sittner et al. [12] have studied the tension-torsion behavior of CuAlZnMn shape memory alloys, under box- and triangle-shaped stress and strain control paths. Lim and McDowell [13] have presented experimental data on a polycrystalline NiTi response to a circular axial-shear strain path. Helm [14,15] has presented extensive biaxial tests on box- and butterfly-shaped strain controlled experiments, while Bouvet et al [16,17] have investigated internal pressure and bi-compression tests on CuAlBe shape memory alloys. Recently, Grabe and Bruhns [18] have conducted several multiaxial experiments on a polycrystalline NiTi sample within a wide temperature range which show the strong non-linear material response as well as the response path dependencies, highlighting the presence of reorientation processes for complex loading paths.

Considering the experimental observations presented in the cited literature and the fact that several SMA applications undergo non-proportional loadings, it is clear the importance of an effective SMA modeling under arbitrary thermo-mechanical loading conditions, especially for non-proportional situations.

2. SMA MODELLING AT SMALL STRAIN REGIME

Up to now, there have been several attempts to properly reproduce SMA material features in a predictive modeling frame. The resulting models can be in general categorized as either micro, micro-macro or macro.

Description of micro-scale features, such as nucleation, interface motion, twin growth, etc., is the main focus of micro models. They are very useful to understand the fundamental phenomenon, although they are not easily applicable at the structural scale. On the other hand, micro-macro studies combine micromechanics and macroscopic thermodynamics to derive constitutive laws of the material. The predictions by these approaches are successful, but the corresponding time-consuming computations make them inappropriate for engineering applications. Finally, phenomenological or macro approaches use the principles of continuum thermodynamics with internal variables to describe the material behavior and, in general, once cast within numerical methods such as the Finite Element Method (FEM), they are suitable for the analysis of SMA-based devices. In the following, we focus on a phenomenological macro modeling approach.

Regarding reorientation phenomenon, several models have recently been proposed by Thiebaud et al. [10], Bouvet et al [16,17], Panico and Brinson [19], Thamburaja [20] , Moumni et al. [21] and Arghavani et al. [22,23].

Selecting an appropriate set of internal variables as macroscopic consequences of the micro-structural changes is the first fundamental issue of phenomenological modeling [24]. In fact, introduction and definition of such internal variables would play a crucial role in arriving at a physically sound constitutive formulation with a simple and consistent structure. Since internal variables are related to micro-structural mechanisms, the definition of their evolution equations is the second fundamental issue of phenomenological modeling and they should be well established with relevant physical considerations [24].

Focusing on shape memory alloys, since the martensitic phase transformation is the basic micro-structural property, in order to incorporate the growth, orientation and reorientation of variants, an appropriate set of internal variables should be able to represent at least a scalar and a directional information. So, on one hand, a set of scalar variables is not adequate for a simple description of the material behavior due to the loss of explicit directional information, while, on the other hand, models that have used tensorial internal variables seem to be more successful since they explicitly include simple directional information. In most of the previously proposed models, inelastic strain has been considered as a unique internal variable; following these approaches, in general, the norm of the inelastic strain represents the scalar martensite amount and its direction represents the preferred direction of the variants. Accordingly, in this class of models scalar and directional informations are tightly interconnected, possibly leading to a somehow more limited or constrained modeling approach.

To give more freedom, in the present work a set of internal variables proposed in [22] is used to propose a general constitutive model with an emphasis on reorientation. A measure of the amount of stress-induced martensite is chosen as a scalar internal variable, being related to the amount of inelastic strain due to stress-induced phase transformation, while the average direction of different variants (or preferred direction of variants) is chosen as a tensorial internal variable, representing the inelastic strain direction. So, using a standard literature terminology [13,16,17] the internal variables may be clearly interpreted as phase transformation and variant reorientation; in this way, transformation and reorientation can be hopefully described with more flexibility.

2.1 Constitutive modeling

According to [22], we select as internal variables a measure of the preferred direction of variants along with the amount of martensite. Assuming small strains, we use the additive strain decomposition:

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^{e} + \boldsymbol{\varepsilon}^{ie} \tag{1}$$

where $\boldsymbol{\varepsilon}$, $\boldsymbol{\varepsilon}^{e}$ and $\boldsymbol{\varepsilon}^{ie}$ are the total, elastic and inelastic strain, respectively. We now introduce a scalar internal variable q defined as $q = \|\boldsymbol{\varepsilon}^{ie}\|$ and a tensorial internal variable $\mathbf{N}$ such that:

$$\boldsymbol{\varepsilon}^{ie} = q\mathbf{N} \tag{2}$$

Moreover, it is required that $0 \le q \le \varepsilon_L$ and $\|\mathbf{N}\| = 1$, where $\|\cdot\|$ is the usual Euclidean norm and ε_L is a material parameter corresponding to the maximum transformation strain reached at the end of the transformation during a uni-axial test.

The model assumes the total strain $\boldsymbol{\varepsilon}$ and the absolute temperature Tas control variables, the norm of inelastic strain q and the average direction of martensite variants $\mathbf{N}$ as internal variables. Introducing the standard decomposition into volumetric and deviatoric part: $\boldsymbol{\varepsilon} = \theta / 3\mathbf{1} + \mathbf{e}$, where $\theta = tr(\boldsymbol{\varepsilon})$ and $\mathbf{e}$ is the deviatoric part of $\boldsymbol{\varepsilon}$, while $\mathbf{1}$ is the second-order identity tensor, the free energy density function Ψ for a polycrystalline SMA material is then expressed as the convex potential [3,4,25,26]:

$$\Psi(\theta, \mathbf{e}, T, q, \mathbf{N}) = \frac{1}{2}K\theta^2 + G\|\mathbf{e} - q\mathbf{N}\|^2 + \tau_M(T) + \frac{1}{2}hq^2 + I_{0,\varepsilon_L}(q) + \kappa(\|\mathbf{N}\| - 1) \tag{3}$$

where *K* and *G* are respectively the bulk and the shear modulus, $\tau_M(T) = \beta\langle T - T_0 \rangle$ with β a material parameter related to the dependency of the critical stress on the temperature, T_0 is the reference temperature and *h* defines the hardening of the phase transformation. Moreover, we make use of the indicator function:

$$I_{0,\varepsilon_L}(q) = \begin{cases} 0 & if \ \ 0 \le q \le \varepsilon_L \\ +\infty & otherwise \end{cases} \tag{4}$$

in order to satisfy the inequality constraint on *q*. The Lagrange multiplier κ has been introduced to satisfy the equality constraint $\|\mathbf{N}\| = 1$. We have also made use of the positive part function $\langle \cdot \rangle$. Starting from the adopted free energy function Ψ and following standard arguments, we can derive the constitutive equations

$$\begin{cases} p = \dfrac{\partial \Psi}{\partial \theta} = K\theta \\ \mathbf{s} = \dfrac{\partial \Psi}{\partial \mathbf{e}} = 2G(\mathbf{e} - \mathbf{e}^{ie}) \\ \eta = -\dfrac{\partial \Psi}{\partial T} = -q\dfrac{\tau_M(T)}{|T - T_0|} \\ Q = -\dfrac{\partial \Psi}{\partial q} = \mathbf{s} : \mathbf{N} - (\tau_M(T) + hq + \gamma) \\ \mathbf{X} = -\dfrac{\partial \Psi}{\partial \mathbf{N}} = q\mathbf{s} - \kappa\mathbf{N} \\ K = -\dfrac{\partial \Psi}{\partial \kappa} = -\|\mathbf{N}\| + 1 = 0 \end{cases} \tag{5}$$

where

$$p = \frac{tr(\boldsymbol{\sigma})}{3}, \qquad \mathbf{s} = \boldsymbol{\sigma} - p\mathbf{1} \tag{6}$$

The quantities $\boldsymbol{\sigma}$, *p*, **s**, η are respectively the Cauchy stress tensor, the volumetric or hydrostatic stress, the deviatoric part of the stress and the entropy. The thermodynamic stress-like quantities *Q* and **X** are associated to the internal variables *q* and **N**. The variable γ results from the indicator function subdifferential $\partial I_{0,\varepsilon_L}(q)$ and it is defined as:

$$\partial I_{0,\varepsilon_L}(q) = \begin{cases} \gamma_1 \le 0 & if \ \ q = 0 \\ 0 & if \ \ 0 < q < \varepsilon_L \\ \gamma_2 \ge 0 & if \ \ q = \varepsilon_L \end{cases} \tag{7}$$

According to (5), the mechanical dissipation inequality reduces to

$$D^{mech} = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - (\dot{\Psi} + \eta\dot{T}) = Q\dot{q} + \mathbf{X} : \dot{\mathbf{N}} \ge 0 \tag{8}$$

In order to satisfy the second law of thermodynamics and the mechanical dissipation inequality (8), we choose the following flow rules for internal variables:

$$\begin{cases} \dot{q} = \dot{\zeta} Q = \dot{\zeta}\left[\mathbf{s} : \mathbf{N} - (\tau_M + hq + \gamma)\right] \\ \dot{\mathbf{N}} = \dot{\lambda}\mathbf{X} = \dot{\lambda}(q\mathbf{s} - \kappa\mathbf{N}) \end{cases} \tag{9}$$

where $\dot{\zeta}$ and $\dot{\lambda}$ are non-negative consistency parameters. From equation $(5)_6$ we may conclude that $\mathbf{N} : \dot{\mathbf{N}} = 0$. Moreover double contracting both sides of equation $(9)_2$ with $\mathbf{N}$ and applying constraint, we can compute the Lagrange multiplier κ as $\kappa = q\mathbf{s} : \mathbf{N}$ and the thermodynamic force $\mathbf{X}$ reads as:

$$\mathbf{X} = q[\mathbf{s} - (\mathbf{s} : \mathbf{N})\mathbf{N}] = q\mathbf{Y} \tag{10}$$

where $\mathbf{Y} = \mathbf{s} - (\mathbf{s} : \mathbf{N})\mathbf{N}$ is the stress component normal to $\mathbf{N}$. Now, we may redefine evolution equations as follows:

$$\begin{cases} \dot{q}\mathbf{N} = \dot{\zeta} Q\mathbf{N} = \dot{\zeta}[Q\mathbf{N} + k(q)\mathbf{Y}] \\ q\dot{\mathbf{N}} = \dot{\lambda}\mathbf{Y} \end{cases} \tag{11}$$

In order to describe phase transformation and reorientation evolution, we choose two limit functions F^{tr} and F^{re} defined as:

$$\begin{cases} F^{tr} = \left\| Q\mathbf{N} + k(q)\mathbf{Y} \right\| - R^{tr}(q) \\ F^{re} = \left\| \mathbf{Y} \right\| - R^{re}(q) \end{cases} \tag{12}$$

where $R^{tr}(q)$ represents the radius of the elastic domain and $R^{re}(q)$ controls the evolution direction of inelastic strain; in the expression of F^{tr}, the term $k(q)$ reflects the effect of reorientation on transformation. The limit function F^{re} affects reorientation by controlling the component of stress normal to the preferred direction of variants and the limit function F^{tr} affects transformation by controlling the transformation thermodynamic force components $Q\mathbf{N}$ in the preferred direction of variants, $\mathbf{N}$, and $k(q)\mathbf{Y}$ normal to that direction.

Also, for generality we can assume that transformation affects reorientation and define an interaction function $\overline{k}(q)$ which leads to redefined evolution equations as:

$$\begin{cases} \dot{q} = \dot{\zeta} Q \\ q\dot{\mathbf{N}} = \left(\dot{\lambda} + \overline{k}(q)\dot{\zeta}\right)\mathbf{Y} \end{cases} \tag{13}$$

We derived the evolution equations and the limit functions for a general case considering the effects of reorientation on transformation through $k(q)$ and using $\overline{k}(q)$ to account for the effects of transformation on reorientation. We now summarize the material law which defines a class of models as follows:

$$\begin{cases} p = K\theta \\ \mathbf{s} = 2G(\mathbf{e}-\mathbf{e}^{ie}) \\ Q = \mathbf{s}:\mathbf{N}-(\tau_M + hq + \gamma) \\ \mathbf{Y} = \mathbf{s}-(\mathbf{s}:\mathbf{N})\mathbf{N} \\ \dot{q} = \dot{\zeta}Q \\ q\dot{\mathbf{N}} = \left(\dot{\lambda}+\bar{k}(q)\dot{\zeta}\right)\mathbf{Y} \\ F^{tr} = \left\|Q\mathbf{N}+k(q)\mathbf{Y}\right\| - R^{tr}(q) \\ F^{re} = \left\|\mathbf{Y}\right\| - R^{re}(q) \\ \dot{\zeta} \geq 0, F^{tr} \leq 0, \dot{\zeta}F^{tr} = 0 \\ \left(\dot{\lambda}+\bar{k}(q)\dot{\zeta}\right) \geq 0, F^{re} \leq 0, \dot{\lambda}F^{re} = 0 \end{cases} \tag{14}$$

To decide on the form of interaction functions $k(q)$ and $\bar{k}(q)$ together with $R^{tr}(q)$ and $R^{re}(q)$, experimental observations should be considered.

2.2 Identification and comparison of some models belonging to the general class

Model 1. This model, elaborated by Auricchio and Petrini [26] from the original model of Souza et al. [25] is characterized by a simple reorientation mechanism and can be considered as a particular member of the introduced class of models, obtained for:

$$k(q) = 1, \quad \bar{k}(q) = 1, \quad R^{tr}(q) = R^{tr}, \quad R^{re}(q) \to +\infty \tag{15}$$

According to (15), we conclude that the limit function F^{re} is always negative which results in $\dot{\lambda} = 0$. In other words, in Model 1 this surface is never activated. Also this model considers the effect of reorientation on transformation $\left(k(q) \neq 0\right)$ and since it is assumed that $\bar{k}(q) \neq 0$ reorientation is affected by transformation.

Model 2. This model, discussed by Arghavani [23], can be interpreted either as an extension of Model 1 (including a more flexible description of reorientation mechanism) or as a modification of the model presented by Panico and Brinson [19]. This model is also a particular member of the general class of models previously discussed, obtained for:

$$k(q) = 1, \quad \bar{k}(q) = 1, \quad R^{tr}(q) = R^{tr}, \quad R^{re}(q) = R^{re} \tag{16}$$

A saturation limit for the component of stress normal to the direction $\mathbf{N}$ is present, but similar to Model 1, orientation is affected by transformation $\left(\bar{k}(q) \neq 0\right)$.

Model 3. This model, proposed by Arghavani et al, [22] is a member of the general class introduced before, but no effect on reorientation due to transformation is considered. The model is obtained for:

$$k(q)=1, \quad \bar{k}(q)=0, \quad R^{tr}(q)=R^{tr}, \quad R^{re}(q)=R^{re} \tag{17}$$

The evolution equations and limit functions for the three models are:

- *Model 1*

$$\begin{cases} \dot{q}=\dot{\zeta}Q \\ q\dot{\mathbf{N}}=\dot{\zeta}\mathbf{Y} \\ F^{tr}=\left\|Q\mathbf{N}+\mathbf{Y}\right\|-R^{tr} \end{cases} \tag{18}$$

- *Model 2*

$$\begin{cases} \dot{q}=\dot{\zeta}Q \\ q\dot{\mathbf{N}}=\left(\dot{\zeta}+\dot{\lambda}\right)\mathbf{Y} \\ F^{tr}=\left\|Q\mathbf{N}+\mathbf{Y}\right\|-R^{tr} \\ F^{re}=\left\|\mathbf{Y}\right\|-R^{re} \end{cases} \tag{19}$$

- *Model 3*

$$\begin{cases} \dot{q}=\dot{\zeta}Q \\ q\dot{\mathbf{N}}=\dot{\lambda}\mathbf{Y} \\ F^{tr}=\left\|Q\mathbf{N}+\mathbf{Y}\right\|-R^{tr} \\ F^{re}=\left\|\mathbf{Y}\right\|-R^{re} \end{cases} \tag{20}$$

The interesting point is that, all of the above mentioned differences appear only for non-proportional loading. In the case of proportional loading, $\mathbf{N}=\mathbf{s}/\left\|\mathbf{s}\right\|$, $\mathbf{Y}=\mathbf{0}$ and $\dot{\lambda}=0$, so Models 1-3 as well as any other model of the proposed class reduce to:

$$\begin{cases} \dot{q}=\dot{\zeta}Q \\ F^{tr}=\left|Q\right|-R^{tr} \end{cases} \tag{21}$$

Figures 1 and 2 compares the model predictions with experimental data.

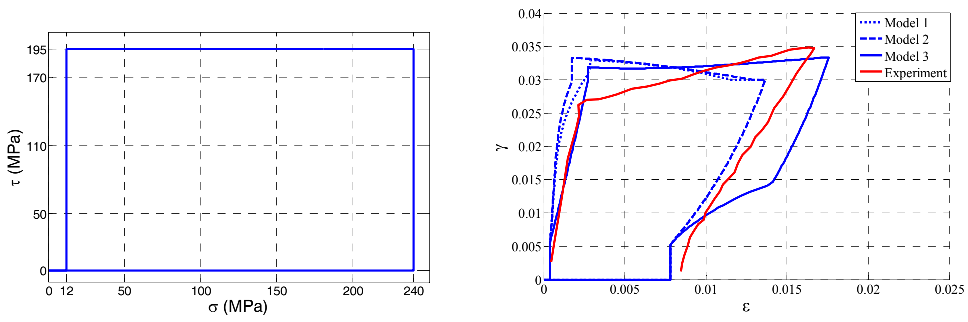

Figure 1: Comparison between models prediction and experimental [12]; non-proportional biaxial tension-shear path (left) b) comparison of predictions between model 1, 2 and 3 and experimental data (right).

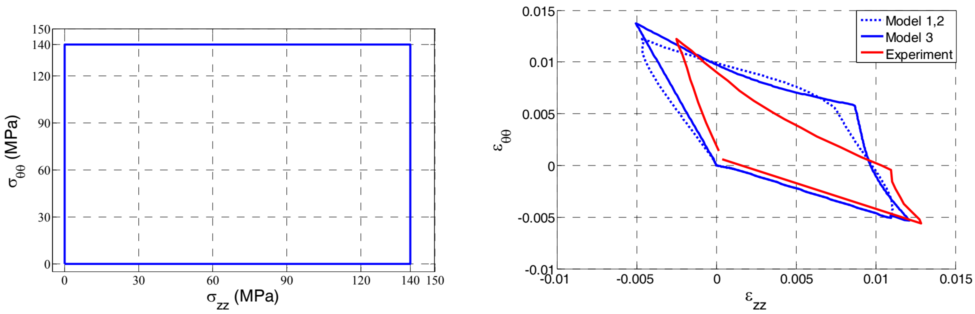

Figure 2: Simulation of the non-proportional biaxial loading; loading path (left) and comparison of models predictions and experimental data [16,17] (right).

2.3 Models in terms of the tensorial internal variable $\mathbf{e}^{ie}$

Most models available in the literature use $\mathbf{e}^{in}$ as internal variable. To present the proposed model in the mentioned well-known form, we substitute q with $\|\mathbf{e}^{ie}\|$ and $\mathbf{N}$ with $\mathbf{e}^{ie}/\|\mathbf{e}^{ie}\|$ in the equations. We specifically present two models in terms of $\mathbf{e}^{in}$. One is the model proposed by Souza et al. [25] and another one, the recently proposed model by Panico and Brinson [19] which are summarized in Tables 1 and 2, respectively.

Table 1: small strain model proposed by Souza et al. [3,4,25,26].

External Variables: $\boldsymbol{\varepsilon}, T$

Internal Variables: $\boldsymbol{\varepsilon}^{ie}$

Stress quantities:

$$p = K\theta, \quad \mathbf{s} = 2G(\mathbf{e} - \mathbf{e}^{ie}), \; \mathbf{X} = s - (\tau_M + h\|\mathbf{e}^{ie}\| + \gamma)\frac{\mathbf{e}^{ie}}{\|\mathbf{e}^{ie}\|}$$

With

$$\begin{cases} \gamma \geq 0 & if \;\; \|\mathbf{e}^{ie}\| = \varepsilon_L \\ \gamma = 0 & if \;\; \|\mathbf{e}^{ie}\| < \varepsilon_L \end{cases}$$

Evolution equation:

$$\dot{\mathbf{e}}^{ie} = \dot{\zeta}\frac{\mathbf{X}}{\|\mathbf{X}\|}$$

Limit function:

$$f = \|\mathbf{X}\| - R$$

Kuhn-Tucker conditions:

$$f \leq 0, \quad \dot{\zeta} \geq 0, \quad \dot{\zeta} f = 0$$

We remark that, in extracting the second model, we assume different limit functions in forward and reverse transformations and since the limit function contains logarithmic terms, it guarantee that always $\|\mathbf{e}^{ie}\| < \varepsilon_L$ and consequently $\gamma = 0$ for ever. We also consider only stress-induced martensite transformation in the original model proposed by Panico and Brinson [19].

Remark: In this study, we use one variable in several models. We highlight that, the variable definition in each part depends on the subject, but it is clear from the context.

Table 2: Small strain model proposed by Panico and Brinson [3,4,25,26].

External Variables: $\boldsymbol{\varepsilon}, T$
Internal Variables: $\boldsymbol{\varepsilon}^{ie}$
Stress quantities:
$p = K\theta, \quad \mathbf{s} = 2G(\mathbf{e}-\mathbf{e}^{ie}), \ \mathbf{X} = s-(\tau_M + h\Vert \mathbf{e}^{ie}\Vert), \mathbf{Y} = s-(s:\mathbf{N})\,\mathbf{N} \ , \ \mathbf{N} = \frac{\mathbf{e}^{ie}}{\Vert \mathbf{e}^{ie}\Vert}$
Evolution equation:
$\dot{\mathbf{e}}^{ie} = \dot{\zeta}\frac{\mathbf{X}}{\Vert \mathbf{X}\Vert} + \dot{\mu}\frac{\mathbf{Y}}{\Vert \mathbf{Y}\Vert}$
Limit functions:
$f^{tr} = \Vert \mathbf{X}\Vert - R^{tr}, \ R^{tr} = \begin{cases} A^f z - B^f z\ln(1-z) + C^f & \text{if } \dot{z} > 0 \\ A^r(1-z) - B^r(1-z)\ln(z) + C^r & \text{if } \dot{z} < 0 \end{cases}$
$f^{re} = \Vert \mathbf{Y}\Vert - R^{re} \quad \text{with} \quad z = \frac{\Vert \mathbf{e}^{ie}\Vert}{\varepsilon_L}$
Kuhn-Tucker conditions:
$f^{tr} \le 0, \ \ \dot{\zeta} \ge 0, \ \ \dot{\zeta} f^{tr} = 0, \quad f^{re} \le 0, \ \ \dot{\mu} \ge 0, \ \ \dot{\mu} f^{re} = 0$

3. SMA MODELLING AT FINITE STRAIN REGIME

Finite strain SMA constitutive models available in the literature has been mainly developed by extending small strain constitutive models. The approach in most of the cases is based on the multiplicative decomposition of the deformation gradient into an elastic and an inelastic or transformation part [27-34], although there are some models in the literature which utilize an additive decomposition of the strain rate tensor into an elastic and an inelastic part [35].

In this work, we first develop a finite-strain SMA model by extending a small-strain constitutive model proposed by Souza et al. [25], its capability in capturing both superelasticity and shape memory effect as well as variant reorientation under multiaxial loadings has been shown in several works by Auricchio and Petrini [3,4,26]. The small-strain model is capable in predicting both superelasticy and shape memory effect as well as variant reorientation under non-proportional loading; it also has a suitable form which makes it possible to develop a robust integration algorithm as well as a successful computational tool. We then, briefly discuss the finite strain extension of the small strain model proposed by Panico and Brinson [19].

Remark: in the finite strain formulation we use superscript “t” in place of “ie” which represents phase transformation.

Considered a deformable body, we denote with **F** the deformation gradient and with J its determinant, supposed to be positive. The tensor **F** can be uniquely decomposed as:

$$\mathbf{F} = \mathbf{RU} = \mathbf{VR} \tag{22}$$

where **U** and **V** are the right and left stretch tensors, respectively, both positive definite and symmetric, while **R** is a proper orthogonal rotation tensor. The right and left Cauchy-Green deformation tensors are then respectively defined as:

$$\mathbf{C} = \mathbf{F}^T\mathbf{F},\ \mathbf{b} = \mathbf{F}\mathbf{F}^T \tag{23}$$

and the Green-Lagrange strain tensor, **E**, reads as:

$$\mathbf{E} = \frac{\mathbf{C} - \mathbf{1}}{2} \tag{24}$$

where $\mathbf{1}$ is the second-order identity tensor. The second Piola-Kirchhoff stress tensor $\mathbf{S}$ is obtained from the Cauchy stress as:

$$\mathbf{S} = J\mathbf{F}^{-1}\sigma\mathbf{F}^{-T} \tag{25}$$

Following a well-stablished approach adopted in plasticity, we assume a local multiplicative decomposition of the deformation gradient into an elastic part $\mathbf{F}^e$, defined with respect to an intermediate configuration, and a transformation one $\mathbf{F}^t$, defined with respect to the reference configuration. Accordingly:

$$\mathbf{F} = \mathbf{F}^e\mathbf{F}^t \tag{26}$$

Since experimental evidences indicate that the transformation flow is nearly isochoric, we have to impose $\det\left(\mathbf{F}^t\right) = 1$, which after taking the time derivative results in $tr(\mathbf{d}^t) = 0$.

We define $\mathbf{C}^e = \mathbf{F}^{eT}\mathbf{F}^e$ and $\mathbf{C}^t = \mathbf{F}^{tT}\mathbf{F}^t$ as the elastic and the transformation right Cauchy-Green tensors and, using definition (23) and (26), we obtain:

$$\mathbf{C}^e = \mathbf{F}^{t-T}\mathbf{C}\mathbf{F}^{t-1} \tag{27}$$

In order to satisfy the principle of material objectivity, the Helmholtz free energy has to depend on $\mathbf{F}^e$ only through the elastic right Cauchy-Green strain tensor; it is moreover assumed to be a function of the transformation strain, $\mathbf{E}^t = (\mathbf{C}^t - \mathbf{1})/2$, and of the temperature in the following form:

$$\Psi = \Psi\left(\mathbf{C}^e, \mathbf{E}^t, T\right) = W(\mathbf{C}^e) + \psi(\mathbf{E}^t, T) \tag{28}$$

where, $W(\mathbf{C}^e)$ is a hyperelastic strain energy function. In addition, we assume $W(\mathbf{C}^e)$ to be an isotropic function of $\mathbf{C}^e$ and to be the same for austenite and martensite phases; we also define ψ in the following form [28,32,33]

$$\psi(\mathbf{E}^t, T) = \tau_M \| \mathbf{E}^t \| + \frac{1}{2} h \| \mathbf{E}^t \|^2 + \mathrm{I}_{\varepsilon_L}(\| \mathbf{E}^t \|) \quad (29)$$

Following standard arguments, the finite strain model [28,32] is summarized in Table 3.

Moreover, recently we have improved the finite strain constitutive model as discussed in the next sections.

3.1 Presenting well- defined, non-singular variables

We note that the variable **N** is not defined for the case of vanishing transformation strain. Despite some discussions in [26], regularization schemes have extensively been used in the literature to overcome this problem. For example Helm and Haupt [15] propose the following regularization scheme:

$$\overline{\| \mathbf{E}^t \|} = \sqrt{\| \mathbf{E}^t \|^2 + \delta} - \delta \quad (30)$$

Table 3: Finite strain extension of constitutive model proposed by Souza et al [28,32].

External Variables: $\mathbf{C}, T$
Internal Variables: $\mathbf{C}^t$
Stress quantities:
$\mathbf{S} = 2\left(\alpha_1 \mathbf{C}^{t-1} + \alpha_2 \mathbf{C}^{t-1}\mathbf{C}\mathbf{C}^{t-1}\right),\ \mathbf{X} = h\mathbf{E}^t + \left(\tau_M + \gamma\right)\mathbf{N},\ \mathbf{Y} = \mathbf{C}\mathbf{S} - \mathbf{C}^t\mathbf{X}$
With
$\begin{cases} \gamma \geq 0 & if\ \| \mathbf{E}^t \| = \varepsilon_L \\ \gamma = 0 & if\ \| \mathbf{E}^t \| < \varepsilon_L \end{cases},\quad \mathbf{N} = \frac{\mathbf{E}^t}{\| \mathbf{E}^t \|}$
$\alpha_1 = \frac{\lambda}{4}\left(\mathbf{C} : \mathbf{C}^{t-1} - 3\right) - \frac{1}{2}\mu, \quad \alpha_2 = \frac{1}{2}\mu$
Evolution equation:
$\dot{\mathbf{C}}^t = 2\dot{\zeta} \frac{\mathbf{Y}^D}{\| \mathbf{Y}^D \|} \mathbf{C}^t$
Limit function:
$f = \| \mathbf{Y}^D \| - R$
Kuhn-Tucker conditions:
$f \leq 0, \quad \dot{\zeta} \geq 0, \quad \dot{\zeta} f = 0$
Norm operator:
$\| \mathbf{Y}^D \| = \sqrt{\mathbf{Y}^D : \mathbf{Y}^{DT}}$

where δ is a user defined parameter (typical value: 10^{-7}). In Auricchio and Petrini [3,4] and adopted also in [28], another proposed regularization scheme is as follows:

$$\overline{\| \mathbf{E}^t \|} = \| \mathbf{E}^t \| - \frac{d^{\frac{d+1}{d}}}{d-1}\left(\| \mathbf{E}^t \| + d\right)^{\frac{d-1}{d}} \tag{31}$$

where d is again a user defined parameter (typical value:0.02). Both regularization schemes (30) and (31) are indeed equivalent, despite they have different forms.

While using a regularization scheme has some advantages in removing the singularity in $\mathbf{N}$ and in giving a smooth transition from austenitic to martensitic phase and vice versa, with a quite simple approach it has however the disadvantage of transforming a large part of the elastic region into a region of nonlinear material response. This has the disadvantage of significantly increased solution time and consequently decreased numerical efficiency, especially for boundary value problems in which a considerable part of the structure remains elastic (as e.g., in stent structures).

We suggest to avoid using a regularized form for $\| \mathbf{E}^t \|$ but to deal with the case of vanishing transformation strain through a careful analytical study of the limiting conditions. The tensor **N** and consequently the tensor **X** are then well-defined, non-singular and continuous through the following definition [32]:

$$\mathbf{N} = \begin{cases} \dfrac{(\mathbf{CS}_e)^D}{\| (\mathbf{CS}_e)^D \|} & \text{if } \| \mathbf{E}^t \| = 0 \\[2ex] \dfrac{\mathbf{E}^t}{\| \mathbf{E}^t \|} & \text{if } \| \mathbf{E}^t \| \neq 0 \end{cases} \tag{32}$$

3.2 Presenting a fully symmetric constitutive model

We observe that due to the asymmetry of **CS**, the quantity **Y** is not symmetric. The asymmetric tensor **Y** also appears in the constitutive equations proposed in [8,28,32,34]. To this end, we present an alternative formulation which is in terms of symmetric tensors only. We may write:

$$\mathbf{CS} = 2\left(\alpha_1 \mathbf{CC}^{t-1} + \alpha_2 \left(\mathbf{CC}^{t-1}\right)^2 + \alpha_3 \left(\mathbf{CC}^{t-1}\right)^3\right) \tag{33}$$

Equation (33) shows that the asymmetry in **CS** is due to the asymmetric term $\mathbf{CC}^{t^{-1}}$. We now present the following identity

$$\mathbf{CC}^{t^{-1}} = \mathbf{U}^t \left(\mathbf{U}^{t^{-1}} \mathbf{C} \mathbf{U}^{t^{-1}}\right) \mathbf{U}^{t^{-1}} = \mathbf{U}^t \overline{\mathbf{C}} \mathbf{U}^{t^{-1}} \tag{34}$$

where

$$\overline{\mathbf{C}} = \mathbf{U}^{t^{-1}} \mathbf{C} \mathbf{U}^{t^{-1}} \tag{35}$$

Substituting (34) into (33), we obtain the proposed improved time-continuous finite-strain constitutive model in Table 4. in [33], it is shown how the improved, symmetric model can improve the computational efficiency.

Table 4: Improved finite strain constitutive model [33].

External Variables: $\mathbf{C}, T$

Internal Variables: $\mathbf{C}^t$

Stress quantities:

$$\mathbf{S} = \mathbf{U}^{t^{-1}} \overline{\mathbf{S}} \mathbf{U}^{t^{-1}}, \ \overline{\mathbf{S}} = 2\left(\alpha_1 \mathbf{1} + \alpha_2 \overline{\mathbf{C}}\right), \ \mathbf{Q} = \overline{\mathbf{C}}\overline{\mathbf{S}} - \mathbf{C}^t \mathbf{X}, \ \mathbf{X} = h\mathbf{E}^t + \left(\tau_M + \gamma\right)\mathbf{N}$$

With

$$\begin{cases} \gamma \geq 0 & if \ \| \mathbf{E}^t \| = \varepsilon_L \\ \gamma = 0 & if \ \| \mathbf{E}^t \| < \varepsilon_L \end{cases}, \quad \mathbf{N} = \begin{cases} \dfrac{\left(\mathbf{Q}_e\right)^D}{\| \left(\mathbf{Q}_e\right)^D \|} & \text{if } \| \mathbf{E}^t \| = 0 \\ \dfrac{\mathbf{E}^t}{\| \mathbf{E}^t \|} & \text{if } \| \mathbf{E}^t \| \neq 0 \end{cases}$$

$$\alpha_1 = \frac{\lambda}{4}\left(\overline{\mathbf{C}} : \mathbf{1} - 3\right) - \frac{1}{2}\mu, \quad \alpha_2 = \frac{1}{2}\mu, \ \overline{\mathbf{C}} = \mathbf{U}^{t^{-1}} \mathbf{C} \mathbf{U}^{t^{-1}}, \ \mathbf{Q}_e = 2\left(\alpha_1 \mathbf{C} + \alpha_2 \mathbf{C}^2\right)$$

Evolution equation:

$$\dot{\mathbf{C}}^t = 2\dot{\zeta} \mathbf{U}^t \frac{\mathbf{Q}^D}{\| \mathbf{Q}^D \|} \mathbf{U}^t$$

Limit function:

$$f = \| \mathbf{Q}^D \| - R$$

Kuhn-Tucker conditions:

$$f \leq 0, \quad \dot{\zeta} \geq 0, \quad \dot{\zeta} f = 0$$

Norm operator:

$$\| \mathbf{Q}^D \| = \sqrt{\mathbf{Q}^D : \mathbf{Q}^D}$$

3.3 Finite strain extension of the small- strain model [19]

In this section, we briefly address the finite strain extension of Panico and Brinson model [19] and refer the reader to [31] for more detail.

In this case, the finite strain model development needs specific considerations. Fore example, motivated by the work by Reese and Christ [34], it may be seems to use a multiplicative decomposition of the deformation gradient into elastic and inelastic parts as well as the decomposition of the inelastic deformation gradient into transformation and reorientation parts. But, this decomposition does not consider the physical assumptions and following this approach can not yield the finite strain extension of the model. To this end, we should consider the physical meaning of the additive decomposition of the inelastic strain rate into transformation and reorientation parts in the small strain regime. Following the physical concepts in the small strain regime, we have used the multiplicative decomposition of the deformation gradient into elastic and inelastic parts together with the additive decomposition of the strain rate tensor into reorientation and transformation parts, i.e.,:

$$\mathbf{F} = \mathbf{F}^e\mathbf{F}^{ie} \quad \text{and} \quad \mathbf{d}^{ie} = \mathbf{d}^{tr} + \mathbf{d}^{re} \tag{35}$$

We report the finite strain constitutive model in Table 5 and refer the reader to Arghavani et al. [31] for more detail. Moreover, we highlight that, following the approach suggested in Section 3.2. it is possible to present a fully symmetric constitutive model for the model summarized in Table 5.

Table 5: Finite strain extension of Panico-Brinson model [31].

External Variables: $\mathbf{C}, T$
Internal Variables: $\mathbf{C}^t$
Stress quantities:
$\mathbf{S} = 2\left(\alpha_1\mathbf{C}^{t-1} + \alpha_2\mathbf{C}^{t-1}\mathbf{C}\mathbf{C}^{t-1}\right), \quad \mathbf{X} = h\mathbf{E}^t + \tau_M\mathbf{N}$
$\mathbf{Y} = \mathbf{CS} - \mathbf{C}^t\mathbf{X}, \quad \mathbf{Z} = \mathbf{CS}, \quad \mathbf{W} = \tilde{\mathbb{I}} : \mathbf{Z}^D$
With
$\alpha_1 = \frac{\lambda}{4}\left(\mathbf{C} : \mathbf{C}^{t-1} - 3\right) - \frac{1}{2}\mu, \quad \alpha_2 = \frac{1}{2}\mu$
Evolution equation:
$\dot{\mathbf{C}}^t = \left(2\dot{\zeta}\frac{\mathbf{Y}^D}{\lVert\mathbf{Y}^D\rVert} + 2\dot{\mu}\frac{\mathbf{W}}{\lVert\mathbf{W}\rVert}\right)\mathbf{C}^t$
Limit functions:
$f^{tr} = \lVert\mathbf{Y}^D\rVert - R^{tr}, \quad R^{tr} = \begin{cases} A^f z - B^f z\ln(1-z) + C^f & \text{if } \dot{z} > 0 \\ A^r(1-z) - B^r(1-z)\ln(z) + C^r & \text{if } \dot{z} < 0 \end{cases}$
$f^{re} = \lVert\mathbf{W}\rVert - R^{re} \quad \text{with} \quad z = \frac{\lVert\mathbf{E}^t\rVert}{\varepsilon_L}$
Kuhn-Tucker conditions:
$f \le 0, \quad \dot{\zeta} \ge 0, \quad \dot{\zeta} f = 0$
Norm operator:
$\lVert\mathbf{Y}^D\rVert = \sqrt{\mathbf{Y}^D : \mathbf{Y}^{DT}}, \quad \lVert\mathbf{W}\rVert = \sqrt{\mathbf{W} : \mathbf{W}^T}$

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