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A THREE-DIMENSIONAL PHENOMENOLOGICAL MODEL FOR SHAPE MEMORY ALLOYS

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Abstract: *Literature presents numerous constitutive models that describe the phenomenological features of the thermomechanical behavior of shape memory alloys (SMAs). The present paper introduces a novel three-dimensional constitutive model that describes the martensitic phase transformations within the scope of standard generalized materials. The model is capable of describing the main features of the thermomechanical behavior of SMAs by considering four macroscopic phases associated with austenitic phase and three variants of martensite. A numerical procedure is proposed to deal with the nonlinearities of the model. Numerical simulations are carried out dealing with uniaxial and multiaxial single-point tests showing the capability of the introduced model to describe the general behavior of SMAs.*

Keywords: *Shape memory alloys, constitutive model, pseudoelasticity.*

1. INTRODUCTION

Shape memory alloys (SMAs) belong to the class of smart materials being used in different kinds of applications, see e.g. Lagoudas (2008), Paiva & Savi (2006), Machado & Savi (2003) and Kalamkarov & Kolpakov (1997). The remarkable properties of SMAs are associated with thermoelastic martensitic transformations that are responsible for different kinds of complex thermomechanical behavior of these smart materials. Besides pseudoelastic and shape memory effects, SMAs may demonstrate interesting behavior as internal subloops due to incomplete phase transformations, two-way shape memory effect, plasticity, transformation induced plasticity, rate-dependency, thermomechanical couplings among other interesting effects related to non-homogeneous characteristics. All these phenomena give a general idea about the complex thermomechanical behavior of SMAs, as discussed by Matsumoto *et al.* (1987), Shaw & Kyriakides (1995), Otsuka & Ren (1999), Gall & Sehitoglu (1999), Patoor *et al.* (2006), Lagoudas *et al.* (2006) and Lagoudas (2008).

The modeling and simulation of thermomechanical behavior of SMAs is the objective of numerous research efforts. The macroscopic modeling is related to phenomenological features, and it relies on the continuum thermodynamics with internal state variables to take into account the changes in the microstructure due to phase transformation (Popov & Lagoudas, 2007; Paiva & Savi, 2006). Paiva & Savi (2006) and Lagoudas (2008) have presented a general overview of the SMA modeling, with the emphasis on the phenomenological constitutive models.

The SMA modeling becomes even more complex when three-dimensional media is of concern. Although many constitutive models are developed for a three-dimensional description, their verification is difficult due to the lack of experimental data. Therefore, many articles in literature present three-dimensional models but only discuss results related to the uniaxial tests. Besides the thermomechanical modeling of SMAs, some experimental reports are of a great importance in order to validate the three-dimensional models. Among other efforts, one could refer to some experimental multiaxial tests performed in different contexts: Grabe & Bruhns (2007); McNaney *et al.* (2007); Manach & Favier (1997); Sittner *et al.* (1995).

The present work proposes a three-dimensional constitutive model developed within the framework of continuum mechanics and generalized standard materials being built upon the classical Fremond's model (Fremond, 1996). The model is inspired on the one-dimensional model that is able to describe different thermomechanical behaviors of SMAs in a flexible way, and its numerical simulations are in a close agreement with the experimental uniaxial tests (Savi *et al.*, 2002; Baêta-Neves *et al.*, 2004; Paiva *et al.*, 2005; Savi & Paiva, 2005; Monteiro Jr *et al.*, 2009). Numerical simulations are carried out for both uniaxial and multiaxial tests considering a single point analysis that shows that the introduced model is able to capture the general thermomechanical behavior of SMAs.

2. CONSTITUTIVE EQUATIONS

Modeling of SMA behavior can be done within the scope of standard generalized materials under the assumption that the thermodynamic state of the material can be completely defined by a finite number of state variables, see e.g. Lemaitre & Chaboche (1990). Under this assumption, the thermomechanical behavior can be described by the Helmholtz free energy density, Ψ, and the pseudo-potential of dissipation, Φ.

Experimental studies have revealed the main aspects of the thermomechanical behavior of SMAs. Basically, there are two possible phases: austenite and martensite. In martensitic phase, different deformation orientations of crystallographic plates constitute what is known by the martensitic variants. In the case of three-dimensional medium, there are 24 possible martensitic variants that are arranged in 6 plate groups with 4 plate variants per group. Because the crystal structure of martensite is less symmetric than the austenite, only a single variant is created on the reverse transformation (Zhang *et al.*, 1991; Schroeder & Wayman, 1977).

The three-dimensional description of thermomechanical behavior of SMAs is usually inspired on one-dimensional models employing a limited number of martensitic variants. Motivated by one-dimensional models, the proposed model considers four macroscopic phases: austenite (A), the twinned martensite (M), which is stable in the absence of a stress field, and two other martensitic phases ($M+$ and $M-$). The definition of the Helmholtz free energy density considers different expressions for each one of the macroscopic phases, assuming that they are functions of strain, ε_{ij}, and temperature, T.

$$
\begin{aligned}
&M^+ : \rho\Psi_1(\varepsilon_{ij}^e,T)=\frac{1}{2}\left(\lambda^M(\varepsilon_{kk}^e)^2+2\mu^M\varepsilon_{ij}^e\varepsilon_{ij}^e\right)-\alpha\Gamma-\Lambda_M-\Omega_{ij}^M(T-T_0)\varepsilon_{ij}^e\\
&M^- : \rho\Psi_2(\varepsilon_{ij}^e,T)=\frac{1}{2}\left(\lambda^M(\varepsilon_{kk}^e)^2+2\mu^M\varepsilon_{ij}^e\varepsilon_{ij}^e\right)+\alpha\Gamma-\Lambda_M-\Omega_{ij}^M(T-T_0)\varepsilon_{ij}^e\\
&A : \rho\Psi_3(\varepsilon_{ij}^e,T)=\frac{1}{2}\left(\lambda^A(\varepsilon_{kk}^e)^2+2\mu^A\varepsilon_{ij}^e\varepsilon_{ij}^e\right)-\Lambda_A-\Omega_{ij}^A(T-T_0)\varepsilon_{ij}^e\\
&M = \rho\Psi_4(\varepsilon_{ij}^e,T)=\frac{1}{2}\left(\lambda^M(\varepsilon_{kk}^e)^2+2\mu^M\varepsilon_{ij}^e\varepsilon_{ij}^e\right)+\Lambda_M-\Omega_{ij}^M(T-T_0)\varepsilon_{ij}^e
\end{aligned}
\tag{1}
$$

Here the indices M and A are related to the martensitic and austenitic phases, respectively; λ and μ are the Lamé coefficients; α is a scalar parameter related to the hysteresis loop; In Eq.(1), Λ_M and Λ_A are temperature functions that define the stress level of phase transformation; Ω_{ij} is a tensor related to the thermal expansion coefficients; T_0 is a reference temperature where free stress state is free of strain; finally, ρ is the material density. Moreover,

$$\Gamma=\frac{1}{3}\varepsilon_{kk}^e+\frac{2}{3}\sqrt{3}\left|\sqrt{J_2^e}\right|\mathrm{sign}(\varepsilon_{kk}^e) \tag{2}$$

where J_2 is a measurement of equivalent strain given by:

$$J_2^e=\frac{1}{6}[(\varepsilon_{22}^e-\varepsilon_{22}^e)^2+(\varepsilon_{22}^e-\varepsilon_{33}^e)^2+(\varepsilon_{33}^e-\varepsilon_{11}^e)^2+3((\varepsilon_{12}^e)^2+(\varepsilon_{21}^e)^2+(\varepsilon_{13}^e)^2+(\varepsilon_{31}^e)^2+(\varepsilon_{23}^e)^2+(\varepsilon_{32}^e)^2)] \tag{3}$$

$\varepsilon_{kk}^e=\varepsilon_{11}^e+\varepsilon_{22}^e+\varepsilon_{33}^e$ and $\mathrm{sign}(\varepsilon_{kk}^e)$ is defined as follows:

The variable Γ can be understood as an equivalent strain field that contributes to phase transformations. Its definition takes into account that phase transformations may be induced either by volumetric expansion (represented by the first term, $\varepsilon_{kk}^e/3$) or by deviatoric effect (represented by the second term, $(2\sqrt{3}/3)\left|\sqrt{J_2^e}\right|\mathrm{sign}(\varepsilon_{kk}^e)$). This hypothesis is based on experimental observations that show that both effects induce phase transformation. It is important to highlight experimental torsion tests that indicate that stress-strain curves are qualitatively similar to those obtained in tensile tests (Jackson *et al.*, 1972; Manach & Favier, 1997; Aguiar *et al.*, 2010). Under this assumption, the equivalent field Γ may be interpreted as a phase transformation inductor that defines what kind of martensitic variant is induced. On the one hand, if $\Gamma \geq 0$ the variant $M+$ is induced. On the other hand, the variant $M-$ is induced when $\Gamma < 0$. Note that each variant can be induced either by volumetric or by shear effects, allowing a proper description of the three-dimensional behavior. Moreover, it should be pointed out that, since the sign of shear strains does not appear in this inductor, they have a neutral influence, tending to follow the volumetric expansion influence. Besides, note that for one-dimensional case, $\Gamma=\varepsilon_{11}^e$, reducing the model to the original one-dimensional description (Savi *et al.*, 2002; Paiva *et al.*, 2005; Aguiar *et al.*, 2010).

In this moment, it is necessary to define the free energy density of the mixture, setting the volume fraction of martensite variants, β_1 and β_2, associated with detwinned martensite (M^+ and M^-, respectively) and β_3, related to austenite (A). The fourth phase is associated with twinned martensite (M) and their volume fraction is β_4.

$$\rho\Psi(\varepsilon_{ij}^e, T, \beta_1, \beta_2, \beta_3, \beta_4) = \rho\sum_{n=1}^{4}\beta_n\Psi_n(\varepsilon_{ij}^e, T) + I_\Theta \tag{4}$$

where $I_\Theta = I_\Theta(\beta_1, \beta_2, \beta_3, \beta_4)$ is the indicator function associated with the convex set Θ (Rockafellar, 1970) that establishes the phase coexistence conditions

$$\Theta = \left\{ \beta_n \in \Re, \left| \begin{array}{l} 0 \le \beta_n \le 1\ (n = 1,2,3,4); \quad \beta_1 + \beta_2 + \beta_3 + \beta_4 = 1 \\ \beta_1 = \beta_2 = 0 \quad \text{if} \quad \sigma_{ij} = 0 \quad \text{and} \quad \beta_1^s = \beta_2^s = 0 \end{array} \right. \right\} \tag{5}$$

From these conditions, it is possible to use $\beta_4 = 1 - \beta_1 - \beta_2 - \beta_3$ in order to define a free energy density in terms of only three volume fractions:

$$\rho\Psi(\varepsilon_{ij}^e, T, \beta_1, \beta_2, \beta_3) = \rho[\beta_1(\Psi_1 - \Psi_4) + \beta_2(\Psi_2 - \Psi_4) + \beta_3(\Psi_3 - \Psi_4) + \Psi_4] + I_\pi \tag{6}$$

Here, the indicator function $I_\pi = I_\pi(\beta_1, \beta_2, \beta_3)$ is related to the convex set π defined as follows:

$$\pi = \left\{ \beta_m \in \Re, \left| \begin{array}{l} 0 \le \beta_m \le 1\ (m = 1,2,3); \quad \beta_1 + \beta_2 + \beta_3 \le 1 \\ \beta_1 = \beta_2 = 0 \quad \text{in stress-free state when } \beta_1^s = \beta_2^s = 0 \end{array} \right. \right\} \tag{7}$$

where β_1^s and β_2^s are the values of β_1 and β_2, respectively, when the phase transformation begins to take place. This is geometrically represented by a tetrahedron in the (β_1, β_2, β_3)-space, shown in Fig. 1.

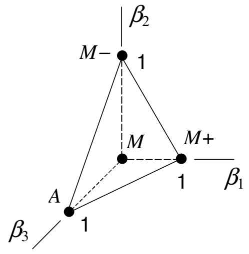

Figure 1. Tetrahedron of the constraints π.

Therefore, the free energy density of the mixture has the following form:

$$\begin{aligned} \rho\Psi(\varepsilon_{ij}^e, T, \beta_1, \beta_2, \beta_3) &= \Gamma\alpha(\beta_2 - \beta_1) - \Lambda(\beta_1 + \beta_2) + \\ &+ \left(\frac{1}{2}(\lambda^A - \lambda^M)(\varepsilon_{kk}^e)^2 + (\mu^A - \mu^M)\varepsilon_{ij}^e\varepsilon_{ij}^e\right)\beta_3 - (\Omega_{ij}^A - \Omega_{ij}^M)(T - T_0)\varepsilon_{ij}^e\beta_3 - \Lambda_3\beta_3 \\ &+ (\frac{1}{2}\lambda^M(\varepsilon_{kk}^e)^2 + \mu^M\varepsilon_{ij}^e\varepsilon_{ij}^e) - \Omega_{ij}^M(T - T_0)\varepsilon_{ij}^e + \Lambda_M + I_\pi \end{aligned} \tag{8}$$

where $\Lambda = 2\Lambda_M$ and $\Lambda_3 = \Lambda_M + \Lambda_A$ .The elastic strain is defined by establishing an additive decomposition given by:

$$\varepsilon_{ij}^e = \varepsilon_{ij} + (\beta_2 - \beta_1)\alpha_{ij}^h \text{sign}(\varepsilon_{kk}^e) \tag{9}$$

where parameter α_{ij}^h is responsible for the horizontal size of the hysteresis loop is stress-strain diagram, being defined as follows:

$$\alpha_{ij}^h = \frac{\sigma^{\max}}{|\sigma^{\max}|}\alpha^h \tag{10}$$

where $\sigma^{\max}$ represents the maximum value of the stress components during a loading process. Moreover, it should be highlighted that $\alpha_{ij}^{h}=0$ if $\sigma^{\max}=0$.

From the generalized standard material approach, the thermodynamical forces associated with each internal variable are defined as follows (Lemaitre & Chaboche, 1990):

$$\sigma_{ij}(\varepsilon_{ij}^{e},T,\beta_1,\beta_2,\beta_3)=\rho\frac{\partial\Psi}{\partial\varepsilon_{ij}^{e}}=\lambda\varepsilon_{ij}^{e}\delta_{ij}+2\mu\varepsilon_{ij}^{e}+\alpha\omega_{ij}(\beta_2-\beta_1)-\Omega_{ij}(T-T_0) \tag{11}$$

$$B_1\in-\rho\partial_{\beta_1}\Psi=\Gamma\alpha+\Lambda+K_1-\alpha_{ij}^{h}\Omega_{ij}(T-T_0)-\partial_{\beta_1}I_\pi \tag{12}$$

$$B_2\in-\rho\,\partial_{\beta_2}\Psi=-\Gamma\alpha+\Lambda-K_2+\alpha_{ij}^{h}\Omega_{ij}(T-T_0)-\partial_{\beta_1}I_\pi \tag{13}$$

$$B_3\in-\rho\,\partial_{\beta_3}\Psi=\Lambda_3+K_3+\left(\Omega_{ij}^{A}-\Omega_{ij}^{M}\right)\alpha_{ij}^{h}(T-T_0)-\partial_{\beta_3}I_\pi \tag{14}$$

where

$$K_1=E_{ijkl}\alpha_{ij}^{h}\varepsilon_{ij}^{e}+(\beta_2-\beta_1)\alpha\left[\frac{1}{3}\alpha_{kk}^{h}+\frac{\left[\left(\alpha_{ii}^{h}-\alpha_{jj}^{h}\right)\left(\varepsilon_{ii}^{e}-\varepsilon_{jj}^{e}\right)+6\left(\alpha_{ij}^{h}\varepsilon_{ij}^{e}-\alpha_{kk}^{h}\varepsilon_{kk}^{e}\right)\right]\text{sign}\,(\varepsilon_{kk}^{e})}{6\sqrt{3J_2^{e}}}\right] \tag{15}$$

$$K_2=-E_{ijkl}\alpha_{ij}^{h}\varepsilon_{ij}^{e}-(\beta_2-\beta_1)\alpha\left[\frac{1}{3}\alpha_{kk}^{h}+\frac{\left[\left(\alpha_{ii}^{h}-\alpha_{jj}^{h}\right)\left(\varepsilon_{ii}^{e}-\varepsilon_{jj}^{e}\right)+6\left(\alpha_{ij}^{h}\varepsilon_{ij}^{e}-\alpha_{kk}^{h}\varepsilon_{kk}^{e}\right)\right]\text{sign}\,(\varepsilon_{kk}^{e})}{6\sqrt{3J_2^{e}}}\right] \tag{16}$$

$$K_3=\left[-\frac{1}{2}\left(\lambda^{A}\left(\varepsilon_{kk}^{h}\right)^2+2\mu^{A}\varepsilon_{ij}^{e}\varepsilon_{ij}^{e}\right)+\frac{1}{2}\left(\lambda^{M}\left(\varepsilon_{kk}^{h}\right)^2+2\mu^{M}\varepsilon_{ij}^{e}\varepsilon_{ij}^{e}\right)\right] \tag{17}$$

Here the $\partial_{\beta_m}(\,)$ represents the subdifferential with respect to β_m. Note that the material parameter is given by a kind of rule of mixtures, being defined as follows:

$$\begin{aligned}\lambda&=\lambda^{M}+\beta_3(\lambda^{A}-\lambda^{M})\\ \mu&=\mu^{M}+\beta_3(\mu^{A}-\mu^{M})\\ \Omega_{ij}&=\Omega_{ij}^{M}+\beta_3(\Omega_{ij}^{A}-\Omega_{ij}^{M})=\Omega\delta_{ij}\end{aligned} \tag{18}$$

It is also important to observe that,

$$\omega_{ij}=\frac{1}{3}\delta_{ij}+\left[\frac{3\varepsilon_{ij}^{e}-\varepsilon_{ij}^{e}\delta_{ij}}{3\sqrt{3J_2^{e}}}\right]\text{sign}\,(\varepsilon_{kk}^{e}) \tag{19}$$

and that $\dfrac{\partial\,\text{sign}(\varepsilon_{kk}^{e})}{\partial\varepsilon_{ij}^{e}}=0$. Moreover, the functions Λ and Λ_3 are temperature dependent and here it is assumed a linear dependence as follows:

$$\Lambda=2\Lambda_M=\begin{cases}-L_0+\dfrac{L}{T_M}(T-T_M) & \text{if}\quad T>T_M\\ -L_0 & \text{if}\quad T\le T_M\end{cases} \tag{20}$$

$$\Lambda_3=\Lambda_M+\Lambda_A=\begin{cases}-L_0^{A}+\dfrac{L^{A}}{T_M}(T-T_M) & \text{if}\quad T>T_M\\ -L_0^{A} & \text{if}\quad T\le T_M\end{cases} \tag{21}$$

where T_M is the temperature below which the martensitic phase becomes stable. Besides, L_0, L, L_0^{A} and L^{A} are parameters related to phase transformation critical stresses. Note that, based on the previous definition, the phase transformation stress level is constant for $T < T_M$.

Since $\lambda\varepsilon_{kk}\delta_{ij}+2\mu\varepsilon_{ij}=E_{ijkl}\varepsilon_{kl}$, it is possible to rewrite the stress-strain relation as follows:

$$\sigma_{ij} = E_{ijkl}\varepsilon_{kl} + \alpha\omega_{ij}(\beta_2 - \beta_1) - \Omega\delta_{ij}(T - T_0) \tag{22}$$

where $E_{ijkl} = E^M_{ijkl} + \beta_3(E^A_{ijkl} - E^M_{ijkl})$. In case of isotropic materials, Lamé coefficients can be expressed in terms of engineering constants as follows:

$$\lambda = \frac{\upsilon E}{(1+\upsilon)(1-2\upsilon)} \quad \text{and} \quad \mu = G = \frac{E}{2(1+\upsilon)} \tag{23}$$

where E is the elastic modulus, G is the shear modulus and υ is the Poison ratio.

The thermomechanical behavior of SMAs is intrinsically dissipative and therefore, it is important to establish the pseudo-potential of dissipation that allows the description of dissipative materials. By assuming that this potential may be split into mechanical and thermal parts, its mechanical part may be considered as follows:

$$\varphi(\dot\beta_1, \dot\beta_2, \dot\beta_3) = \frac{1}{2}(\eta_1\dot\beta_1^2 + \eta_2\dot\beta_2^2 + \eta_3\dot\beta_3^2) + I_x \tag{24}$$

where $I_x = I_x(\dot\beta_1, \dot\beta_2, \dot\beta_3)$ is the indicator function related to the convex set χ, that provides constraints associated with phase transformation evolution. Physically, this indicator function establishes constraints related to internal subloops due to incomplete phase transformations and also to the formation of detwinned martensite (*M*). Hence, for $|\dot\sigma_{ij}| = 0$ the convex set χ can be written as follows:

$$\chi = \left\{ \dot\beta_n \in \Re \left| \begin{array}{l} \dot T\dot\beta_1 \begin{cases} < 0 & \text{if} \quad \dot T > 0, \quad \sigma_{ij} = 0 \quad \text{and} \quad \beta_1^s \neq 0 \\ = 0 & \text{otherwise} \end{cases} \\ \dot T\dot\beta_2 \begin{cases} < 0 & \text{if} \quad \dot T > 0, \quad \sigma_{ij} = 0 \quad \text{and} \quad \beta_2^s \neq 0 \\ = 0 & \text{otherwise} \end{cases} \\ \dot T\dot\beta_3 \geq 0 \\ -\dot\beta_1^2 - \dot\beta_1\dot\beta_3 = 0 \quad \text{or} \quad -\dot\beta_2^2 - \dot\beta_2\dot\beta_3 = 0 \end{array} \right. \right. \tag{25}$$

Together with constraints related to internal subloops, the set (21) also expresses a constraint to eliminate both M+ → M and M− → M phase transformations. In mathematical terms, this is expressed by $\dot\beta_1\dot\beta_4 = \dot\beta_1(-\dot\beta_1 - \dot\beta_2 - \dot\beta_3) = -\dot\beta_1^2 - \dot\beta_1\dot\beta_3 = 0$ or by $\dot\beta_2\dot\beta_4 = \dot\beta_2(-\dot\beta_1 - \dot\beta_2 - \dot\beta_3) = -\dot\beta_2^2 - \dot\beta_2\dot\beta_3 = 0$, respectively, which means that when one kind of transformation occurs the other must vanish. Moreover, the discarded terms in both equations ($-\dot\beta_1\dot\beta_2$) represent impossible transformations and, thus, are not considered. Otherwise, for a system with some kind of mechanical loading $|\dot\sigma_{ij}| \neq 0$:

$$\chi = \left\{ \dot\beta_n \in \Re \left| \begin{array}{l} \dot\Gamma\dot\beta_1 \geq 0; \quad \dot\Gamma\dot\beta_3 \leq 0; \quad \text{if} \quad \Gamma \geq 0 \\ \dot\Gamma\dot\beta_2 \leq 0; \quad \dot\Gamma\dot\beta_3 \geq 0; \quad \text{if} \quad \Gamma < 0 \end{array} \right. \right. \tag{26}$$

Under these assumptions, and considering again the generalized standard materials approach, the thermodynamical fluxes are represented as (Lemaitre & Chaboche, 1990):

$$\partial_{\dot\beta_m}\varphi = \eta_m\dot\beta_m + \partial_{\dot\beta_m} I_\chi = B_m \quad (m = 1,2,3) \text{, without summation} \tag{27}$$

In order to contemplate different aspects of kinetics of phase transformation, parameter η_i may assume different values for cases of loading or unloading behaviors:

$$\begin{cases} \eta_i = \eta_i^L \text{ if } \quad \dot\Gamma \geq 0 \\ \eta_i = \eta_i^U \text{ if } \quad \dot\Gamma < 0 \end{cases} \tag{28}$$

These equations establish a complete set of constitutive relations, given by:

$$\begin{aligned}
&\sigma_{ij} = E_{ijkl}\varepsilon^e_{kl} + (\beta_2 - \beta_1)\alpha\omega_{ij} - \Omega\delta_{ij}(T - T_0) \\
&\dot{\beta}_1 = \frac{1}{\eta_1}\left\{\Gamma\alpha + \Lambda + K_1 - (T - T_0)\alpha^h_{ij}\delta_{ij}\Omega - \partial_{\beta_1} I_\pi\right\} - \partial_{\dot{\beta}_1} I_\chi \\
&\dot{\beta}_2 = \frac{1}{\eta_2}\left\{-\Gamma\alpha + \Lambda - K_2 + (T - T_0)\alpha^h_{ij}\delta_{ij}\Omega - \partial_{\beta_2} I_\pi\right\} - \partial_{\dot{\beta}_2} I_\chi \\
&\dot{\beta}_3 = \frac{1}{\eta_3}\left\{K_3 + \Lambda_3 + (\Omega^A - \Omega^M)(T - T_0)\alpha^h_{ij}\delta_{ij} - \partial_{\beta_3} I_\pi\right\} - \partial_{\dot{\beta}_3} I_\chi
\end{aligned} \tag{30}$$

Nonlinearities of the formulation are treated by considering an iterative numerical procedure based on the operator split technique (Ortiz *et al.*, 1983). The procedure is similar to that employed earlier for the one-dimensional media, see Savi *et al.* (2002) and Paiva *et al.* (2005). The procedure isolates the subdifferentials and uses the implicit Euler method combined with an orthogonal projection algorithm to evaluate evolution equations. Orthogonal projections assure that volume fractions of the martensitic variants obey the imposed constraints. In order to satisfy constraints expressed in Eq. (9), values of volume fractions must stay inside or on the boundary of π, the tetrahedron shown in Fig. 1.

In order to evaluate the capability of the above introduced model to describe thermomechanical behavior of SMAs, numerical results from the uniaxial and multiaxial single-point tests are carried out. Specifically, uniaxial tests show pseudoelasticity, shape memory effect, phase transformation due to temperature variations and internal subloops due to incomplete phase transformations. Concerning multiaxial tests, the pure shear stress and hydrostatic tests are discussed showing qualitatively coherent results. Table 1 presents model parameters employed for all numerical simulations.

Table 1. Model parameters.

$E_A (GPa)$	$E_M (GPa)$	$\alpha (MPa)$	$\Omega_A (MPa/K)$	$\Omega_M (MPa/K)$
54	42	330	0.74	0.17
$L_0 (MPa)$	$L(MPa)$	$L_0^A (MPa)$	$L^A (MPa)$	$T_M (K)$
0.15	41.5	0.63	185	291.4
$T_A (K)$	$\eta^L (MPa.s)$	$\eta^U (MPa.s)$	$\eta_3^L (MPa.s)$	$\eta_3^U (MPa.s)$
307.5	1	2.7	1	2.7
α^h	ν^A	ν^M		
0.0473	0.3	0.44		

3. NUMERICAL SIMULATIONS: UNIAXIAL TESTS

In order to evaluate the capability of the proposed model to describe thermomechanical behavior of SMAs, let us consider uniaxial tests related to a single-point tensile behavior, assuming that $\Gamma = \varepsilon_{11}$ and $\nu = 0$. Initially, the verification of the proposed model is done by comparing numerical simulation with experimental data presented by Tobushi *et al.* (1991), which describes tensile tests on Ni-Ti wires at different temperatures such as 333 *K*, 353 *K* and 373 *K*. Figure 2 presents the comparison showing a good agreement between numerical and experimental tests.

Let us now focus our attention on the shape memory effect. The SMA specimen starts at *T* = 260K, a temperature where martensite is stable, and then is subjected to a mechanical loading. After the loading-unloading process, the specimen is subjected to a temperature change. Figure 3 presents the thermomechanical loading process. At the beginning of the process, the mechanical loading is applied at a low temperature, upon final unloading there is still some residual strain, which can be fully recovered by heating the sample until austenite becomes stable and cooling back to the test temperature. Figure 3 also presents stress-strain-temperature curve showing the complete process and the corresponding volume fraction evolution. Initially, the mechanical loading causes the reorientation from M to M+. Afterwards, the temperature change causes the phase transformation from M+ to A, which is responsible for residual strain recovery.

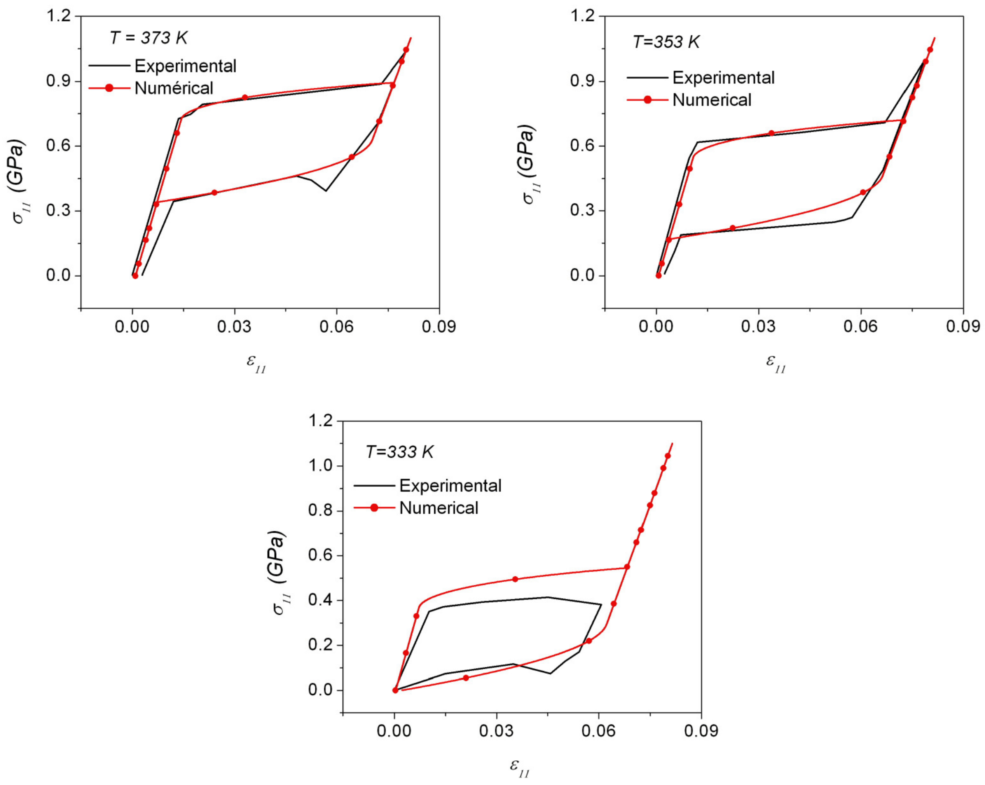

Figure 2. Comparison between numerical and experimental results (Tobushi *et al.*, 1991).

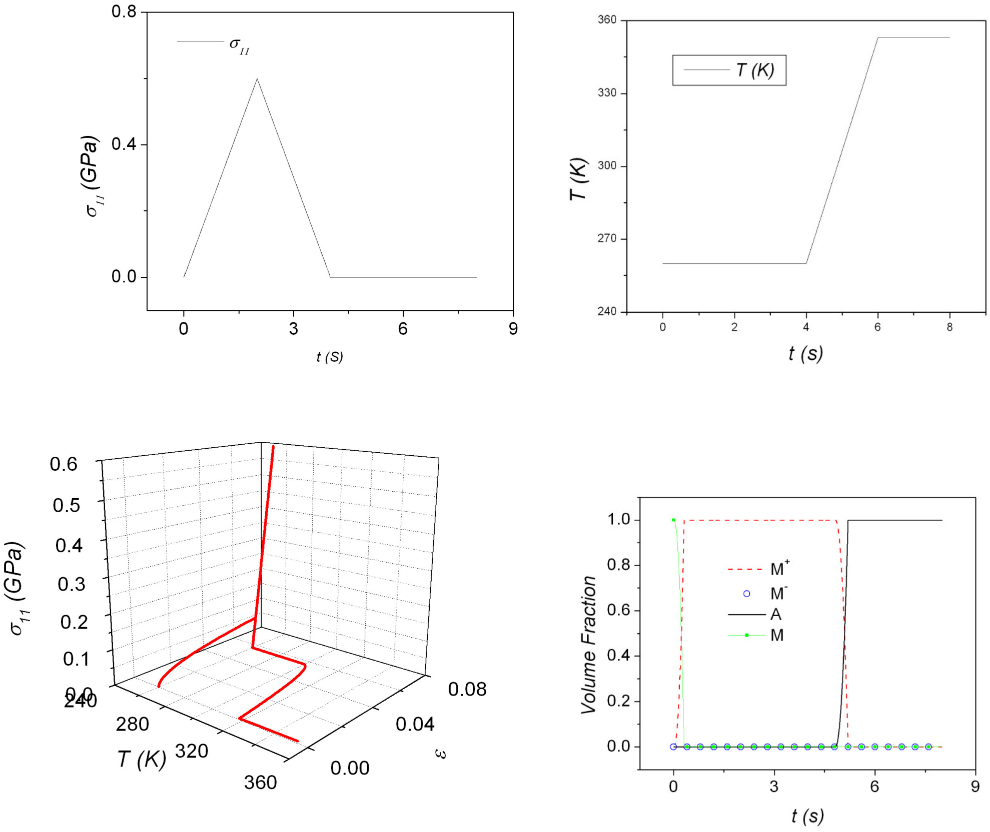

Figure 3. Shape memory effect.

4. NUMERICAL SIMULATIONS: MULTIAXIAL TESTS

This section deals with multiaxial tests that are used to show the capabilities of the above introduced three-dimensional model. Initially, pure shear test is performed in order to verify the consistence of the model. Afterwards, a more complex loading process is of concern.

4.1. Pure Shear Test

The analysis of a pure shear stress test allows us to verify the coordinate invariance by establishing a comparison between the pure shear state with the one with tensile and compressive stress of the same value. Therefore, the maximum values of the stress tensors of these two states are given by:

$$\sigma_{ij}^{A} = \begin{bmatrix} 0.8 & 0 & 0 \\ 0 & -0.8 & 0 \\ 0 & 0 & 0 \end{bmatrix} \text{GPa} \qquad \sigma_{ij}^{B} = \begin{bmatrix} 0 & 0.8 & 0 \\ 0.8 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \text{GPa}$$

Tests are carried out at temperature T = 373K, which coincides with the temperature T_0. Figure 4 shows the SMA response presenting the stress-strain curves and the volume fraction evolution, comparing the following curves: $\sigma_{11}\times\varepsilon_{11}$ and $\sigma_{12}\times\varepsilon_{12}$. The response is a typical pseudoelastic behavior and it is important to note that curves are identical, confirming the system invariance.

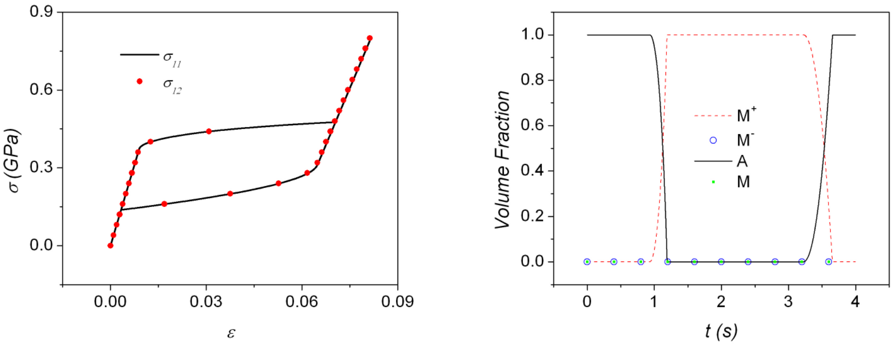

Figure 4. Pure shear test.

4.2. Plane Stress Test

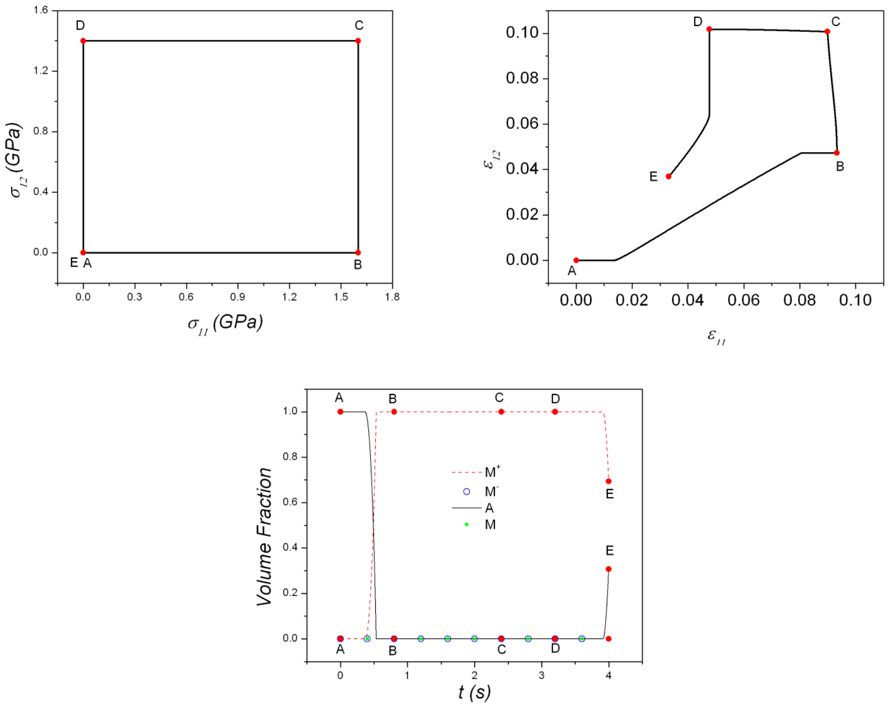

Figure 5. Plane stress test: stress space, strain space and volume fractions.

At this point, an analysis of a plane stress test is of concern. The loading process is shown in Figure 5 representing a situation where a tensile loading is applied with a linear increase until a maximum value is reached. Afterwards, a shear stress is applied with a linear increase, keeping the tensile load constant. Then, similar procedure is adopted in order to remove both loads. Figure 5 also presents the strain space resulting from this loading process. The nonlinearity of the curve is clearly noticeable. Since the shear loading is applied keeping the tensile load constant, great part of the phase transformation is induced when shear load is applied, see volume fraction evolution. It is also important to observe that the positive volume fraction is induced as a consequence of the inductor characteristics ($\Gamma \geq 0$). Figure 6 stress-strain curves related to this process.

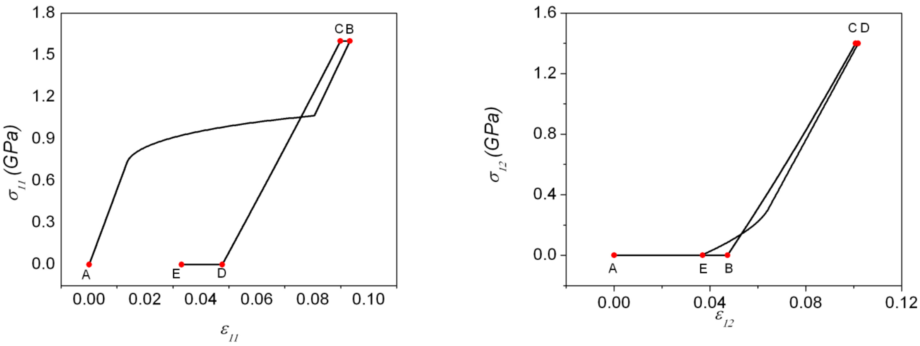

Figure 6. Plane stress test: stress-strain curves.

5. CONCLUSIONS

The present work proposes a novel three-dimensional constitutive model to describe the thermomechanical behavior of shape memory alloys. The phenomenological model is developed within the framework of continuum mechanics and the generalized standard materials. Inspired on one-dimensional models, four macroscopic phases are considered assuming different properties for austenitic and martensitic phases. Martensitic reorientation is defined by an equivalent field that includes either the volumetric expansion or the deviatoric effect. Numerical simulations are carried out for uniaxial and multiaxial single-point tests. Uniaxial tests represent the typical thermomechanical behavior of tensile tests showing pseudoelasticity and shape memory effect. Multiaxial tests are carried out in order to evaluate the capabilities of the introduced model to describe different thermomechanical loadings. Pure shear and plane stress tests are explored showing a qualitative coherence and presenting important characteristics of the model as the coordinate invariance.

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