A ONE-DIMENSIONAL CONSTITUTIVE MODEL FOR SHAPE MEMORY ALLOYS

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Abstract

Shape memory and pseudoelastic effects may be modeled either by microscopic or macroscopic point of view. Phenomenological aspects of SMA behavior are considered by constitutive models which are formulated to describe these phenomena. The present contribution considers a new one-dimensional constitutive model with internal constraint to describe SMA behavior. The proposed theory contemplates four phases: three variants of martensite and an austenitic phase. Two different elastic moduli for austenitic and martensitic phases and new constraints are also conceived for a correct description of phenomena related to SMA. A numerical procedure is developed and numerical results show that the proposed model is capable to describe shape memory and pseudoelastic effects.

Key-words: Shape Memory Alloys, Constitutive Equations.

1. INTRODUCTION

Shape memory alloys (SMAs) are a family of metals with the ability of changing shape depending on their temperature. SMAs undergo thermoelastic martensitic transformations which may be induced either by temperature or stress. When a specimen of SMA is stressed at a constant higher temperature, inelastic deformation is observed above a critical stress. This inelastic deformation, however, fully recovers during the subsequent unloading. The stress-stain curve, which is the macroscopic manifestation of the deformation mechanism of the martensite, forms a hysteresis loop. At a lower temperature, some amount of strain remains after complete unloading. This residual strain may be recovered by heating the specimen. The first case is the pseudoelastic effect, while the last is the shape memory effect (SME) or one way SME. These effects are inter-related in the sense that, if the hysteresis cycle in the pseudoelastic case is not completed when the applied stress is removed, then reversion of the residual martensite must be induced upon heating, by employing the SME (Sun & Hwang, 1993). In the process of returning to their remembered shape, these alloys can generate large forces which may be useful for actuation (Rogers, 1995). Because of such remarkable properties, SMAs have found a number of applications in engineering.

Metallurgical studies have revealed the microstructural aspects of the behavior of SMAs. Basically, there are two possible phases on SMAs: austenite and martensite. In martensitic phase, there are plates which may be internally twin-related. Hence, different deformation orientations of crystallographic plates constitute what is known by martensitic variants. On SMAs there are 24 possible martensitic variants which are arranged in 6 plates groups with 4 plate variants per group (Zhang *et al*., 1991). Schroeder & Wayman (1977) have shown that when a specimen is deformed bellow a temperature where only martensitic phase is stable, with increasing stress, only one of the 4 variants in a given plate group will begin to grow. This variant is the one that has the largest partial shear stress. On the other hand, 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). For one-dimensional cases, it is possible to consider only three variants of martensite on SMAs: the twinned martensite (*M*), which appears with no stress field, and two other martensitic phases (*M*+, *M*-), which are induced by positive and negative stress fields, respectively.

Shape memory alloys may be modeled either by microscopic or macroscopic point of view. Phenomenological aspects of SMA behavior are contemplated by constitutive models which are formulated to describe these phenomena (Birman, 1997). The following classification may be considered to the phenomenological theories: Polynomial models, models based on plasticity, models with internal constraints and model with assumed phase transformation kinetics.

Polynomial model was proposed by Falk (1980) and is based on the Devonshire theory for temperature-induced first order phase transition combined with hysteresis. This is a one-dimensional model that defines a polynomial free energy which describes pseudoelasticity and shape memory in a very simple way.

Models based in plasticity exploit the well-established principles of the theory of plasticity. Bertram (1982) proposes a three-dimensional model using the concepts of kinematics and isotropic hardening. Mamiya and co-workers (Silva, 1995; Souza *et al.*, 1998; Motta *et al.*, 1999) also presents models which are capable to describe shape memory and pseudoelastic effects. Auricchio and co-workers also introduces models using these ideas. First, Auricchio & Lubliner (1997) and Auricchio & Sacco (1997) present a one-dimensional model and then, it is extrapolated to include the analysis in the set of three-dimensional media (Auricchio *et al*., 1997).

Models with assumed transformation kinetics consider that the phase transformation is governed by a known function which is determined through the current values of stress and temperature. The first model based in this formulation was proposed by Tanaka & Nagaki (1982) which originates other models proposed by Liang & Rogers (1990), Brinson (1993), Boyd & Lagoudas (1994), Ivshin & Pence (1994). Perhaps, these are the most popular models to describe SMA behavior.

Models with internal constraints consider internal variables to describe the volumetric fractions of the material phase and constraints, which establishes the form how the phases may coexist. Fremond (1987) develops a three-dimensional model which considers three phases: two variants of martensite and an austenitic phase. Limitations of this theory are discussed in Savi & Braga (1993a). Abeyaratne *et al.* (1994) describes phase transformation kinetics with the aid of some constraints based on thermodynamic admissibility rules. The model of Auricchio and co-workers also may be included in this classification.

The present contribution considers a new one-dimensional constitutive model with internal constraint to describe SMA behavior. The proposed theory is based on Fremond's model and includes four phases in the formulation: three variants of martensite and an austenitic phase. The inclusion of twinned martensite allows one to describe a stable phase when the specimen is at a lower temperature and free of stress. This is an improvement of the proposed model when compared to the original Fremond's model. Furthermore, two different elastic moduli for austenitic and martensitic phases and new constraints are conceived in the formulation. A numerical procedure is developed and numerical results show that the proposed model is capable to describe shape memory and pseudoelastic effects.

2. CONSTITUTIVE MODEL

Fremond (1987) has proposed a three-dimensional model for the thermomechanical response of SMA where martensitic transformations are described with the aid of two internal variables. These variables represent volumetric fractions of two variants of martensite (*M*+ and *M*-), and must satisfy constraints regarding the coexistence of three distinct phases, the third being the parent austenitic phase (*A*). It has been noted (Savi & Braga, 1993a) that Fremond's original model can not present good results in three-dimensional problems, however, one-dimensional results are qualitatively good. Here, an alternative one-dimensional model is considered introducing a fourth variant of martensitic phase: twinned martensite.

SMA behavior can be characterized by the Helmholtz free energy, ψ, and the potential of dissipation, ϕ. The thermodynamic state is completely defined by a finite number of state variables: deformation, ε, temperature, T, the volumetric fractions of martensitic variants, β_1 and β_2, which are associated with detwinned martensites (*M*+ and *M*-) and austenite (*A*), β_3. The fourth phase is associated with twinned martensite (*M*) and its volumetric fraction is β_4. Each phase have a free energy function as follows,

$$M+: \quad \rho\psi_1(\varepsilon,T)=\frac{1}{2}E_M\varepsilon^2-\alpha\varepsilon \tag{1}$$

$$M-: \quad \rho\psi_2(\varepsilon,T)=\frac{1}{2}E_M\varepsilon^2+\alpha\varepsilon \tag{2}$$

$$A: \quad \rho\psi_3(\varepsilon,T)=\frac{1}{2}E_A\varepsilon^2-\frac{L_A}{T_M}(T-T_M) \tag{3}$$

$$M: \quad \rho\psi_4(\varepsilon,T)=\frac{1}{2}E_M\varepsilon^2+\frac{L_M}{T_M}(T-T_M) \tag{4}$$

where α, $L_M=L_M(T)$ and $L_A=L_A(T)$ are material parameters that describe the martensitic transformation, E_M and E_A represents the elastic moduli for the martesitic and austenitic phases, respectively; T_M is a temperature below which the martensitic phase becomes stable in the absence of stress; ρ is the density. A free energy for the mixture can be written as follows,

$$\rho\hat{\psi}(\varepsilon,T,\beta_i)=\rho\sum_{i=1}^{4}\beta_i\psi_i(\varepsilon,T)+\hat{\mathbf{J}}(\beta_i) \tag{5}$$

where the volumetric fraction of the phases must satisfy constraints regarding the coexistence of four distinct phases:

$$\beta_i \geq 0 \quad (i=1,2,3,4)\ ; \quad \beta_1+\beta_2+\beta_3+\beta_4=1 \tag{6}$$

In the absence of strain, the detwinned martensites, *M*+ and *M*-, do not exist. In order to include this physical aspect, an additional constraint must be written,

$$\beta_1 = \beta_2 = 0 \ \text{ if } \varepsilon = 0 \tag{7}$$

With these considerations, $\hat{\mathbf{J}}$ is the indicator function of the convex τ (Rockafellar, 1970):

$$\tau = \left\{\beta_i \in \Re \;\middle|\; 0 \leq \beta_i \leq 1\left(i=1,2,3,4\right); \beta_1+\beta_2+\beta_3+\beta_4=1; \beta_1=\beta_2=0 \ \text{ if } \varepsilon=0\right\} \tag{8}$$

Using constraints (6), β_4 can be eliminated and the free energy can be rewritten as:

$$\rho\psi(\varepsilon,T,\beta_1,\beta_2,\beta_3) = \rho\tilde{\psi}(\varepsilon,T,\beta_1,\beta_2,\beta_3) + \mathbf{J}(\beta_1,\beta_2,\beta_3) \tag{9}$$

where,

$$\begin{aligned}\rho\tilde{\psi}(\varepsilon,T,\beta_1,\beta_2,\beta_3) = {} & \beta_1\left[-\alpha\varepsilon - \frac{L_M}{T_M}(T-T_M)\right] + \beta_2\left[\alpha\varepsilon - \frac{L_M}{T_M}(T-T_M)\right] + \\ & + \beta_3\left[\frac{1}{2}(E_A - E_A)\varepsilon^2 - \frac{L_M+L_A}{T_M}(T-T_M)\right] + \frac{1}{2}E_M\varepsilon^2 + \frac{L_M}{T_M}(T-T_M)\end{aligned} \tag{10}$$

Now, **J** represents the indicator function of the tetrahedron π of the set (Figure 1),

$$\pi = \left\{\beta_i \in \Re \;\middle|\; 0 \leq \beta_i \leq 1\left(i=1,2,3\right); \beta_1+\beta_2+\beta_3 \leq 1; \beta_1=\beta_2=0 \ \text{ if } \varepsilon=0\right\} \tag{11}$$

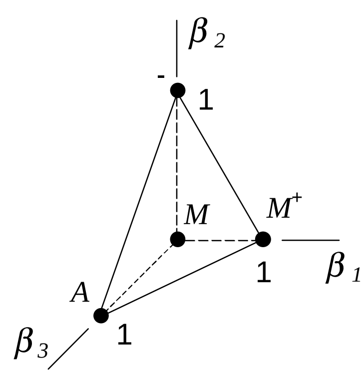


Figure 1 - Tetrahedron of the constraints π.

State equations can be obtained from the Helmholtz free energy as follows:

$$\sigma = \rho \frac{\partial \tilde{\psi}}{\partial \varepsilon} = [E_M - \beta_3 (E_M - E_A)]\varepsilon + \alpha(\beta_2 - \beta_1) \tag{12}$$

$$B_1 \in -\rho \frac{\partial \tilde{\psi}}{\partial \beta_1} - \partial_1 J = \alpha\varepsilon + \frac{L}{T_A}(T - T_A) - \partial_1 J \tag{13}$$

$$B_2 \in -\rho \frac{\partial \tilde{\psi}}{\partial \beta_2} - \partial_2 J = -\alpha\varepsilon + \frac{L_M}{T_M}(T - T_M) - \partial_2 J \tag{14}$$

$$B_3 \in -\rho \frac{\partial \tilde{\psi}}{\partial \beta_3} - \partial_3 J = -\frac{1}{2}(E_M - E_A)\varepsilon^2 + \frac{L_M + L_A}{T_M}(T - T_M) - \partial_3 J \tag{15}$$

where B_i are thermodynamic forces and σ represents the uniaxial stress; ∂_i is the *sub-differential* with respect to β_i (Rockafellar, 1970). Lagrange multipliers offer a good alternative to represent sub-differentials of the indicator function (Savi & Braga, 1993b). Considering a pseudo-potential of dissipation of the following type,

$$\phi(\beta_1, \beta_2, \beta_3) = \frac{\eta}{2}(\dot{\beta}_1^2 + \dot{\beta}_2^2 + \dot{\beta}_3^2) \tag{16}$$

where η is a parameter associated with the internal dissipation of the material, it is possible to write the following complementary equations:

$$B_i = \frac{\partial \phi}{\partial \dot{\beta}_i} = \eta \dot{\beta}_i \quad (i = 1,2,3) \tag{17}$$

These equations form a complete set of constitutive equations. Since the pseudo-potential of dissipation is convex, positive and vanishes at the origin, the Clausius-Duhen inequality (Eringen, 1967), is automatically satisfied if the entropy is defined as $s = -\partial\psi / \partial T$.

Further, it is important to consider the definition of the parameters L_M=$L_M(T)$ and L_A=$L_A(T)$, which is obtained assuming $\dot{\beta}_1 = 0$ and $\varepsilon = \varepsilon_R = \alpha / E_M$ in a critical temperature, T_C, below which there is no residual strain. Hence, using these conditions in Equation (14), one obtains the following expressions,

$$L_M(T) = \begin{cases} L_M = L, & \text{if} \quad T \geq T_C \\ L_M = L \dfrac{(T_C - T_M)}{(T - T_M)}, & \text{if} \quad T < T_C \end{cases} \tag{18}$$

$$L_A(T) = \begin{cases} L_A = L, & \text{if} \quad T \geq T_C \\ L_A = 2L - \left[L \dfrac{(T_C - T_M)}{(T - T_M)} \right], & \text{if} \quad T < T_C \end{cases} \tag{19}$$

In order to solve the governing equations, an algorithm based on the operator split technique (Ortiz *et al.*, 1983) are conceived. The procedure isolates the sub-differentials and uses the implicit *Euler's method* combined with an *orthogonal projection* (Savi & Braga, 1993b) to evaluate evolution equations. Orthogonal projections guarantee that volumetric fractions of the martensitic variants will obey the imposed constraints. In order to satisfy constraints expressed in (6), values of volumetric fractions must stay inside or on the boundary of π, the tetrahedron shown in Figure 1. For instance, if the values of a volumetric fraction calculated by (17) fall outside the region π, the projection are prescribed in such a way that the result will be pulled to the nearest point on the boundary of the tetrahedron.

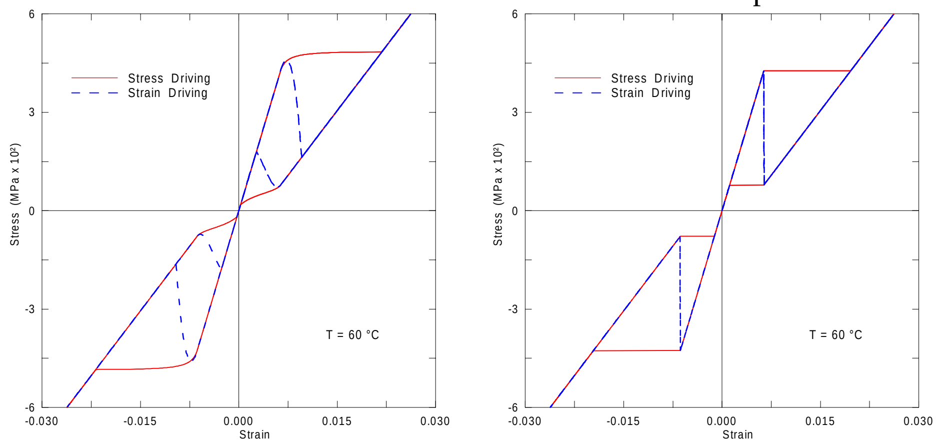
3. NUMERICAL SIMULATIONS

In order to evaluate the response predicted by the proposed model, a SMA specimen which properties are presented in Table 1, is subjected to a thermomechanical loading.

Table 1 - Mechanical properties.

E_A (GPa)	E_M (GPa)	α (GPa)	L (MPa/°C)	T_M (^{0}C)
67.0	26.3	0.228	61.6	18.4

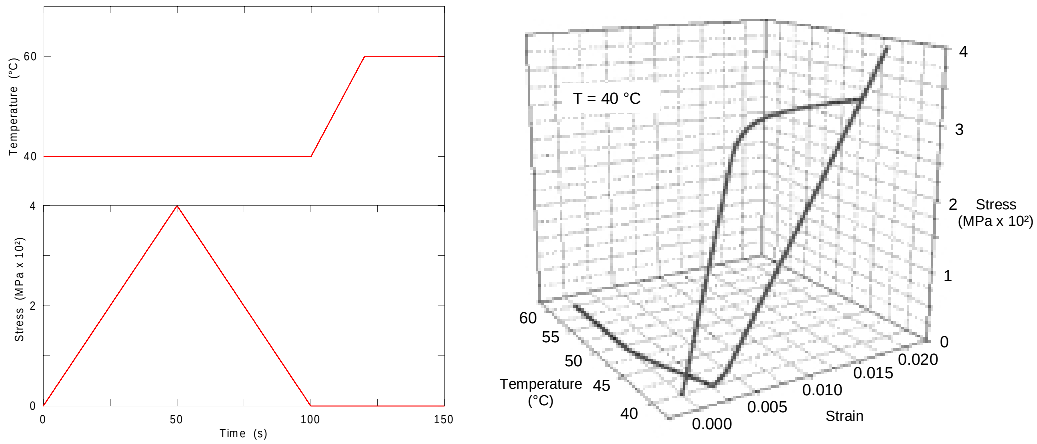
At first, the pseudoelastic effect is contemplated regarding a SMA specimen subjected to a mechanical loading with a constant temperature (T = 60^{0}C). The stress-strain curve for stress and strain driving cases and different values of the parameter η, are presented in Figure 2. Notice that the strain driving case predicts a softening behavior. Further, it should be pointed out that there are two different elastic moduli for the austenitic and martensitic phase.



(a) (b)

Figure 2 - Pseudoelastic effect ($T = 60\,°C > T_A$). (a) $\eta = 7 \times 10^4$ MPa.s; (b) $\eta = 7 \times 10^{-4}$ MPa.s

The shape memory effect is now contemplated regarding a thermomechanical loading depicted in Figure 3a. Firstly, one conceives a constant temperature T = 40^{0}C, where the martensitic phase is stable. The dissipation parameter is η = 7 x 10^4 MPa.s. After mechanical loading-unloading process (Figure 3a), the specimen presents a residual strain that can be eliminated by a subsequent thermal loading (Figure 3a). Notice that the stress-strain-temperature curve (Figure 3b) represents the shape memory effect. Further, it is important to observe that there is a stable phase, associated with the twinned martensite, when the specimen is free of stress.



(a) (b)

Figure 3 - Shape Memory effect.

4. CONCLUSIONS

The present contribution proposes a new one-dimensional constitutive model with internal constraint to describe SMA behavior. The proposed theory considers the twinned martensite in the formulation and, as a consequence, there is a stable phase when the material is free of stress at low temperatures. The consideration of different elastic moduli for austenite and martensite is another improvement of the theory. The inclusion of the constraint which establishes that the detwinned martensites does not exist in the absence of strain, permits to describe thermoelasticity behavior. A numerical procedure is developed and numerical results show that the proposed model are capable to describe shape memory and pseudoelastic effects. Some features are still needed to be contemplated in the proposed model and one could mention the elimination of the softening behavior for strain driving case and also the internal loops observed during cyclic loads associated with incomplete phase transformations.

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