Phenomenological Modeling and Numerical Simulation of Shape Memory Alloys: A Thermo-plastic-phase Transformation Coupled Model

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ABSTRACT: The thermomechanical behavior of shape memory alloys (SMAs) may be modeled either by microscopic or macroscopic point of view. Shape memory, pseudoelasticity and thermal expansion are phenomena related to the SMA behavior. Constitutive models consider phenomenological aspects of these phenomena. The present contribution considers a one-dimensional constitutive model with internal constraint to describe SMA behavior including the effect of plastic strains. The proposed theory contemplates four phases: three variants of martensite and an austenitic phase. Different material parameters for austenitic and martensitic phases are considered. Thermal expansion phenomenon and plastic effects are also contemplated. Hardening effect is represented by a combination of kinematic and isotropic behaviors. A plastic-phase transformation coupling is incorporated into the model. A numerical procedure is developed and numerical results show that the proposed model is capable to capture the general thermomechanical behavior of shape memory alloys.

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–strain curve, which is the macroscopic manifestation of the deformation mechanism of the martensite, forms a hysteresis loop (Figure 1a). At a lower temperature, some amount of strain remains after complete unloading. This residual strain may be recovered by heating the specimen (Figure 1b). The first case is the pseudoelastic effect, while the last is the shape memory effect (SME) or one-way SME. After subjecting the specimen to a training routine, such as a series of SME cycles or a series of stress induced martensite cycles, it is possible to obtain changes in shape in both directions as a function of temperature (heating and cooling). Therefore, both high and low temperature shapes may be remembered. This phenomenon is the two-way SME (Zhang et al., 1991).

Because of such remarkable properties, SMAs have found a number of applications in different fields of sciences and engineering. They are ideally suited for use as fastener, seals, connectors and clamps (Borden, 1991; Kibirkstis et al., 1997; van Humbeeck, 1999). Self-actuating fastener, thermally actuator switches and a number of bioengineering devices are some examples of these applications (Schetky, 1979; Stice, 1990; Airoldi and Riva, 1996; Duerig et al., 1999; Lagoudas et al., 1999). The use of SMAs can help solving many important problems in aerospace technology, in particular those concerning space savings achieved by self-erectable structures, stabilizing mechanisms, solar batteries, nonexplosive release devices and other possibilities (Schetky, 1979; Busch et al., 1992; Denoyer et al., 2000; Pacheco and Savi, 2000). Micromanipulators and robotics actuators have been built employing SMAs to mimic the smooth motions of human muscles (Rogers, 1995; Fujita and Toshiyoshi, 1998; Webb et al., 2000; Garner et al., 2001). Also, SMAs are being used as actuators for vibration and buckling control of flexible structures. In this particular field, SMAs wires embedded in composite materials have been used to modify mechanical characteristics of slender structures (Rogers et al., 1991; Rogers, 1995; Birman et al., 1996; Birman, 1997; Chen and Levy, 1999; Choi et al., 1999; Lee et al., 1999; Pietrzakowski, 2000). The main drawback of SMAs is their slow rate of change.

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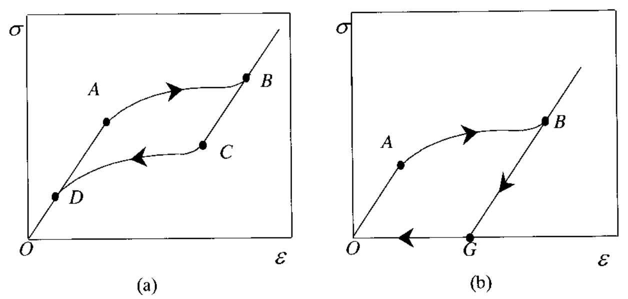


Figure 1. *(a) Pseudoelastic effect; (b) shape memory effect.*

Metallurgical studies have revealed the microstructural aspects of the behavior of SMAs (Shaw and Kyriakides, 1995; Birman, 1997; Otsuka and Ren, 1999). Basically, there are two possible phases on SMAs: austenite and martensite. In martensitic phase, there are plates that 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 plate groups with 4 plate variants per group (Zhang et al., 1991). Schroeder and Wayman (1977) have shown that when a specimen is deformed below 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 is stable in the absence of a stress field, and two other martensitic phases ($M+$, $M-$), which are induced by positive and negative stress fields, respectively.

The thermomechanical behavior of shape memory alloys may be modeled either by microscopic or macroscopic point of view. Constitutive models consider phenomenological aspects of this behavior (Birman, 1997) and, despite the large number of applications, the modeling of SMA is not well-established (James, 2000). The following classification may be considered to the phenomenological theories: Polynomial models, models based on plasticity, model with assumed phase transformation kinetics and models with internal constraints.

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 (Muller and Xu, 1991).

Models based on plasticity exploit the well-established principles of the theory of plasticity. Bertran (1982) proposes a three-dimensional model using the concepts of kinematics and isotropic hardening. Mamiya and coworkers (Silva, 1995; Souza et al., 1998; Motta et al., 1999) present models which are capable to describe shape memory and pseudoelastic effects. Auricchio and coworkers also introduces models using these ideas. First, Auricchio and Lubliner (1997) and Auricchio and 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). Govindjee and Kasper (1997), Leclerq et al. (1995) and Govindjee and Hall (2000) are other references.

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. Tanaka and Nagaki (1982) proposed the first model based on this formulation. This theory originates other models proposed by Liang and Rogers (1990), Brinson (1993), Boyd and Lagoudas (1994), Ivshin and 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, 1996) develops a three-dimensional model, which considers three phases: two variants of martensite and an austenitic phase. Some characteristics of this theory are discussed in Savi and 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 coworkers also may be included in this classification. Another reference is Pagano and Alart (1999).

Other models reported in literature are Achenbach and Muller (1982), Berveiller et al. (1991), Graesser and Cozzarelli (1994), Barret (1995) and Terriault et al. (1997).

Plastic strains are concerned in different articles in order to evaluate either effects of these strains in phase transformations or the description of the two-way shape memory effect (Lim and McDowell, 1994; Fischer et al., 1998; Bo and Lagoudas, 1999; Dobovsek, 2000; Govindjee and Hall, 2000; Lexcellent et al., 2000; Miller and Lagoudas, 2000; Zhang and McCormick, 2000a, b). The loss of actuation through repeated cycling due to plastic strain development is one of the important aspects related to the effect of plastic strains in SMAs.

This article is concerned with a one-dimensional constitutive model with internal constraint to describe SMA behavior. The proposed theory is based on the 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. Furthermore, different material parameters for austenitic and martensitic phases and new constraints are concerned. Thermal expansion and plastic strains are also included into the formulation. Hardening effect is represented by a combination of kinematic and isotropic behaviors. A plastic-phase transformation coupling is incorporated into the model allowing a correct description of the thermomechanical behavior of SMAs. An iterative numerical procedure based on the operator split technique (Ortiz et al., 1983), the orthogonal projection algorithm (Savi and Braga, 1993b) and the return mapping algorithm (Simo and Taylor, 1986; Simo and Hughes, 1998) is developed. Numerical results show that the proposed model is capable to capture the general thermomechanical behavior of shape memory alloys.

CONSTITUTIVE MODEL

Fremond (1987, 1996) 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 that Fremond's original model present qualitatively good results in the description of one-dimensional media (Savi and Braga, 1993a). Here, an alternative one-dimensional model is considered introducing a fourth variant of martensitic phase: twinned martensite.

Modeling of SMA behavior can be done within the scope of the standard generalized material (Lemaitre and Chaboche, 1990). With this assumption, the thermomechanical behavior can be described by the Helmholtz free energy, ψ, and the dual of pseudo-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 $M-$, respectively) and austenite (A), β_3. The fourth phase is associated with twinned martensite (M) and its volumetric fraction is β_4. The plastic phenomenon is described with the aid of plastic strain, ε^p, and the hardening effect is represented by a combination of kinematic and isotropic behaviors, described by variables μ and γ, respectively. Additive decomposition is assumed and the total strain, ε, may be split into a phase transformation part, $\varepsilon^{\mathrm{SMA}}$, usually considered on SMA description, and a plastic part, ε^p.

$$\varepsilon = \varepsilon^{SMA} + \varepsilon^p \tag{1}$$

With these assumptions, each phase have a free energy function as follows,

$$M+: \ \rho\psi_1 = \frac{1}{2}E_M(\varepsilon-\varepsilon^p)^2 - \alpha(\varepsilon-\varepsilon^p) - \Omega_M(T-T_0)(\varepsilon-\varepsilon^p) + \frac{1}{2}K_M\gamma^2 + \frac{1}{2H_M}\mu^2 \tag{2}$$

$$M-: \ \rho\psi_2 = \frac{1}{2}E_M(\varepsilon-\varepsilon^p)^2 + \alpha(\varepsilon-\varepsilon^p) - \Omega_M(T-T_0)(\varepsilon-\varepsilon^p) + \frac{1}{2}K_M\gamma^2 + \frac{1}{2H_M}\mu^2 \tag{3}$$

$$A: \ \rho\psi_3 = \frac{1}{2}E_A(\varepsilon-\varepsilon^p)^2 - \frac{L_A}{T_M}(T-T_M) - \Omega_A(T-T_0)(\varepsilon-\varepsilon^p) + \frac{1}{2}K_A\gamma^2 + \frac{1}{2H_A}\mu^2 \tag{4}$$

$$M: \ \rho\psi_4 = \frac{1}{2}E_M(\varepsilon-\varepsilon^p)^2 + \frac{L_M}{T_M}(T-T_M) - \Omega_M(T-T_0)(\varepsilon-\varepsilon^p) + \frac{1}{2}K_M\gamma^2 + \frac{1}{2H_M}\mu^2 \tag{5}$$

where α, $L_M = L_M(T)$ and $L_A = L_A(T)$ are material parameters that describe martensitic transformation, E_M and E_A represents the elastic moduli for martensitic and austenitic phases, respectively; Ω_M and Ω_A represents the thermal expansion coefficient for martensitic and austenitic phases, respectively; K_M and K_A are the plastic moduli for martensitic and austenitic phases while H_M and H_A are the kinematic hardening moduli martensitic and austenitic phases; T_M is a temperature below which the martensitic phase starts its formation in the absence of stress while T_0 is a reference temperature; ρ is the density. A free energy for the mixture can be written as follows,

$$\rho\hat{\psi}(\varepsilon, T, \beta_i, \varepsilon^p, \gamma, \mu) = \rho \sum_{i=1}^{4} \beta_i\psi_i(\varepsilon, T, \varepsilon^p, \gamma, \mu) + \hat{\mathbf{J}}(\beta_i) \tag{6}$$

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

$$0 \le \beta_i \le 1 \ (i = 1, 2, 3, 4); \ \ \beta_1 + \beta_2 + \beta_3 + \beta_4 = 1 \tag{7}$$

Detwinned martensites, $M+$ and $M-$, are induced by stress fields. In order to include this physical aspect, an additional constraint must be written,

$$\beta_1 = \beta_2 = 0 \quad \text{if } \sigma = 0 \text{ and } \beta_1^S = \beta_2^S = 0 \tag{8}$$

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

$$\tau = \left\{ \beta_i \in \Re \middle| \begin{array}{l} 0 \leq \beta_i \leq 1\ (i=1,2,3,4);\ \beta_1+\beta_2+\beta_3+\beta_4=1; \\ \beta_1=\beta_2=0 \quad \text{if } \sigma=0 \text{ and } \beta_1^S=\beta_2^S=0 \end{array} \right\} \tag{9}$$

Using constraints (7), β_4 can be eliminated and the free energy can be rewritten as:

$$\rho\psi(\varepsilon, T, \beta_1, \beta_2, \beta_3, \varepsilon^p, \gamma, \mu) = \rho\tilde{\psi}(\varepsilon, T, \beta_1, \beta_2, \beta_3, \varepsilon^p, \gamma, \mu) + \mathbf{J}(\beta_1, \beta_2, \beta_3) \tag{10}$$

where,

$$\begin{aligned}
\rho\tilde{\psi} = {} & \beta_1\left[-\alpha(\varepsilon-\varepsilon^p) - \frac{L_M}{T_M}(T-T_M)\right] \\
& + \beta_2\left[\alpha(\varepsilon-\varepsilon^p) - \frac{L_M}{T_M}(T-T_M)\right] \\
& + \beta_3\left[\frac{1}{2}(E_A-E_M)(\varepsilon-\varepsilon^p)^2 - \frac{(L_A+L_M)}{T_M}(T-T_M)\right. \\
& \quad - (\Omega_A-\Omega_M)(T-T_0)(\varepsilon-\varepsilon^p) \\
& \quad \left. + \frac{1}{2}(K_A-K_M)\gamma^2 + \left(\frac{1}{2H_A} - \frac{1}{2H_M}\right)\mu^2\right] \\
& + \frac{1}{2}E_M(\varepsilon-\varepsilon^p)^2 + \frac{L_M}{T_M}(T-T_M) \\
& - \Omega_M(T-T_0)(\varepsilon-\varepsilon^p) + \frac{1}{2}K_M\gamma^2 + \frac{1}{2H_M}\mu^2
\end{aligned} \tag{11}$$

Now, **J** represents the indicator function of the tetrahedron π of the set (Figure 2),

$$\pi = \left\{ \beta_i \in \Re \middle| \begin{array}{l} 0 \leq \beta_i \leq 1\ (i=1,2,3);\ \beta_1+\beta_2+\beta_3 \leq 1; \\ \beta_1=\beta_2=0 \quad \text{if } \sigma=0 \quad \text{and} \quad \beta_1^S=\beta_2^S=0 \end{array} \right\} \tag{12}$$

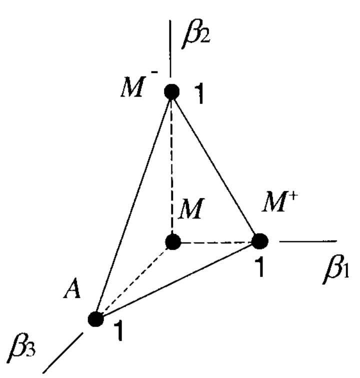


Figure 2. *Tetrahedron of the constraints* Π.

State equations can be obtained from the Helmholtz free energy as follows (Lemaitre and Chaboche, 1990):

$$\sigma = \rho\frac{\partial\psi}{\partial\varepsilon} = E\,(\varepsilon-\varepsilon^p) + \alpha(\beta_2-\beta_1) - \Omega(T-T_0) \tag{13}$$

$$B_1 = -\rho\frac{\partial\psi}{\partial\beta_1} = \alpha(\varepsilon-\varepsilon^p) + \frac{L_M}{T_M}(T-T_M) - \partial_1 J \tag{14}$$

$$B_2 = -\rho\frac{\partial\psi}{\partial\beta_2} = -\alpha(\varepsilon-\varepsilon^p) + \frac{L_M}{T_M}(T-T_M) - \partial_2 J \tag{15}$$

$$\begin{aligned}
B_3 = {} & -\rho\frac{\partial\psi}{\partial\beta_3} = -\frac{1}{2}(E_A-E_M)(\varepsilon-\varepsilon^p)^2 + \frac{L_A+L_M}{T_M}(T-T_M) \\
& + (\Omega_A-\Omega_M)(T-T_0)(\varepsilon-\varepsilon^p) - \frac{1}{2}(K_A-K_M)\gamma^2 \\
& - \left(\frac{1}{2H_A} - \frac{1}{2H_M}\right)\mu^2 - \partial_3 J
\end{aligned} \tag{16}$$

$$X = -\rho\frac{\partial\psi}{\partial\varepsilon^p} = E(\varepsilon-\varepsilon^p) + \alpha(\beta_2-\beta_1) - \Omega(T-T_0) = \sigma \tag{17}$$

$$Y = -\rho\frac{\partial\psi}{\partial\gamma} = -K\gamma \tag{18}$$

$$Z = -\rho\frac{\partial\psi}{\partial\mu} = -\frac{1}{H}\mu \tag{19}$$

where B_i are thermodynamic forces related to SMA behavior, while X, Y and Z are associated with plastic behavior; 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 and Braga, 1993b). Notice that the following definitions was considered in the previous equations:

$$E = E_M - \beta_3(E_M - E_A) \tag{20}$$

$$\Omega = \Omega_M - \beta_3(\Omega_M - \Omega_A) \tag{21}$$

$$K = K_M - \beta_3(K_M - K_A) \tag{22}$$

$$\frac{1}{H} = \frac{1}{H_M} - \beta_3\left(\frac{1}{H_M} - \frac{1}{H_A}\right) \tag{23}$$

Moreover, consider the dual of pseudo-potential of dissipation of the following type,

$$\begin{aligned}
\phi^* = {} & \frac{1}{2\eta}[(B_1 + \eta_{ci}Y + \eta_{ck}Z)^2 + (B_2 + \eta_{ci}Y + \eta_{ck}Z)^2 \\
& + (B_3 - \eta_{ci}Y - \eta_{ck}Z)^2] + I_f
\end{aligned} \tag{24}$$

where I_f is the indicator function related to the yield surface defined as follows (Lemaitre and Chaboche, 1990),

$$f(X, Z, Y) = |X + HZ| - (\sigma_Y - Y) \quad \text{or} \\ f(\sigma, \mu, \gamma) = |\sigma - \mu| - (\sigma_Y + K\gamma) \tag{25}$$

The parameter η is associated with the internal dissipation of the material while η_{ci} and η_{ck} are related to plastic-phase transformation coupling. The parameter η_{ci} is associated with isotropic hardening coupling while η_{ck} is associated with kinematic hardening. At this point, it is possible to write the following complementary equations (Lemaitre and Chaboche, 1990):

$$\dot{\beta}_1 = \partial_{B_1}\phi^* = \frac{B_1}{\eta} + \frac{\eta_{ci}}{\eta}Y + \frac{\eta_{ck}}{\eta}Z = \frac{B_1}{\eta} - \frac{\eta_{ci}}{\eta}K\gamma - \frac{\eta_{ck}}{\eta}\frac{\mu}{H} \tag{26}$$

$$\dot{\beta}_2 = \partial_{B_2}\phi^* = \frac{B_2}{\eta} + \frac{\eta_{ci}}{\eta}Y + \frac{\eta_{ck}}{\eta}Z = \frac{B_2}{\eta} - \frac{\eta_{ci}}{\eta}K\gamma - \frac{\eta_{ck}}{\eta}\frac{\mu}{H} \tag{27}$$

$$\dot{\beta}_3 = \partial_{B_3}\phi^* = \frac{B_3}{\eta} - \frac{\eta_{ci}}{\eta}Y - \frac{\eta_{ck}}{\eta}Z = \frac{B_3}{\eta} + \frac{\eta_{ci}}{\eta}K\gamma + \frac{\eta_{ck}}{\eta}\frac{\mu}{H} \tag{28}$$

$$\dot{\varepsilon}^p = \partial_X\phi^* = \lambda\,\text{sign}(X + HZ) = \lambda\,\text{sign}(\sigma - \mu) \tag{29}$$

$$\dot{\gamma} = \partial_Y\phi^* = \lambda + \eta_{ci}(\dot{\beta}_1 + \dot{\beta}_2 - \dot{\beta}_3) \\ = |\dot{\varepsilon}^p| + \eta_{ci}(\dot{\beta}_1 + \dot{\beta}_2 - \dot{\beta}_3) \tag{30}$$

$$\dot{\mu} = \partial_Z\phi^* = \lambda H\,\text{sign}(X + HZ) + \eta_{ck}(\dot{\beta}_1 + \dot{\beta}_2 - \dot{\beta}_3) \\ = H\dot{\varepsilon}^p + \eta_{ck}(\dot{\beta}_1 + \dot{\beta}_2 - \dot{\beta}_3) \tag{31}$$

where λ is the classical plastic multiplier. The irreversible nature of plastic flow is represented by means of the *Kuhn–Tucker conditions*. Another constraint must be satisfied when $f(\sigma, \gamma, \mu) = 0$. It is referred as *consistency condition* and corresponds to the physical requirement that a stress point on the yield surface must persist on it. These conditions are presented as follows (Simo and Hughes, 1998):

$$\lambda \geq 0;\ f(\sigma, \gamma, \mu) \leq 0;\ \lambda f(\sigma, \gamma, \mu) \\ \lambda\dot{f}(\sigma, \gamma, \mu) = 0 \quad \text{if } (\sigma, \gamma, \mu) = 0 \tag{32}$$

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 $s = -\partial\psi/\partial T$.

Moreover, 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 $\varepsilon = \varepsilon_R$ in a critical temperature, T_C, below which the value of residual strain remains constant. With this aim, it is necessary to define,

$$\varepsilon_R = \frac{L_M[\alpha + \Omega_M(T_M - T_0)]}{L_M E_M + \alpha\Omega_M T_M} \tag{33}$$

$$T_C = T_M\left[\frac{L_M E_M + \alpha(\Omega_M T_0 - \alpha)}{L_M E_M + \alpha\Omega_M T_M}\right] \tag{34}$$

Hence, one wishes to limit the displacement of the hysteresis loop with respect to temperature when $T < T_C$. With this aim, the term $L_M(T)$ is defined in such a way that $L_M(T)(T - T_M)/(T_M)$ becomes a constant for $T < T_C$. Also, $L_M(T) + L_A(T) = 2L$, and therefore, the following expressions are obtained,

$$L_M(T) = \begin{cases} L_M = L, & \text{if } T \geq T_C \\ L_M = L\dfrac{(T_C - T_M)}{(T - T_M)}, & \text{if } T < T_C \end{cases} \tag{35}$$

$$L_A(T) = \begin{cases} L_A = L, & \text{if } T \geq T_C \\ L_A = 2L - \left[L\dfrac{(T_C - T_M)}{(T - T_M)}\right], & \text{if } T < T_C \end{cases} \tag{36}$$

The parameter L may be evaluated as a function of T_A, a temperature above which austenitic phase starts its formation in the absence of stress, as follows:

$$L = \frac{(E_A + E_M)\varepsilon_R^2}{2(T_A/T_M - 1)} \tag{37}$$

NUMERICAL PROCEDURE

The operator split technique (Ortiz et al., 1983) associated with an iterative numerical procedure is developed in order to deal with the nonlinearities in the formulation. The procedure isolates the subdifferentials and uses the implicit Euler method combined with an orthogonal projection algorithm (Savi and Braga, 1993b) to evaluate evolution equations. Orthogonal projections assure that volumetric fractions of the martensitic variants will obey the imposed constraints. In order to satisfy constraints expressed in Equation (12), values of volumetric fractions must stay inside or on the boundary of π, the tetrahedron shown in Figure 2. For instance, if trial values of volumetric fractions calculated fall outside the region π, $\bar{\beta} = (\bar{\beta}_1, \bar{\beta}_2, \bar{\beta}_3)$, the projection are prescribed in such a

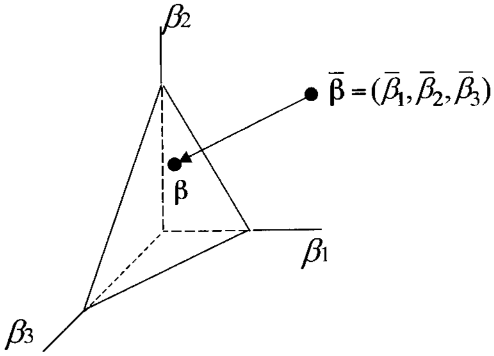


Figure 3. *Orthogonal projection in tetrahedron of the constraints π.*

way that the result will be pulled to the nearest point on the boundary of the tetrahedron, $\beta = (\beta_1, \beta_2, \beta_3)$ (Figure 3).

The elasto-plastic behavior is simulated with the aid of the return mapping algorithm proposed by Simo and Taylor (1986). In this algorithm, a trial state is defined by considering an elastic predictor step, using the implicit Euler algorithm to make the time discretization of evolution equations. If $f_{n+1}^{\text{trial}} \leq 0$, it means that the state is on the elastic domain and the trial state is the actual one. Otherwise, if $f_{n+1}^{\text{trial}} > 0$, we are outside the elastic domain and a plastic step must be considered. Hence, the trial state must be corrected by a projection (Simo and Taylor, 1986; Simo and Hughes, 1998).

NUMERICAL SIMULATIONS

In order to evaluate the response predicted by the proposed model, a SMA specimen with typical properties of a Ni–Ti alloy, is subjected to different thermomechanical loadings. Material properties presented in Table 1 are related to the classical Fremond model for shape memory alloys (Fremond, 1996) and also plastic parameters associated with theory of plasticity (Simo and Hughes, 1998). Stress-driving or temperature-driving simulations are carried out.

The yield limit σ_Y has a linear variation with T, evaluated with the following expression:

$$T \leq T_M \Rightarrow \sigma_Y = \sigma_Y^M \tag{38}$$

$$T_M < T \leq T_A \Rightarrow \sigma_Y = \frac{\sigma_Y^M (T_A - T) + \sigma_Y^{A,i}(T - T_M)}{T_A - T_M} \tag{39}$$

$$T_A < T \leq T_F \Rightarrow \sigma_Y = \frac{\sigma_Y^{A,i} (T_F - T) + \sigma_Y^{A,f}(T - T_A)}{T_F - T_A} \tag{40}$$

where T_F is used to determine the angular coefficient of the linear interpolation.

Table 1. Thermomechanical properties.

E_A (GPa)	E_M (GPa)	α (MPa)	η (MPa/K)		
67	26.30	89.42	0.07		
T_M (K)	T_A (K)	T_0 (K)	Ω_A (MPa/K)	Ω_M (MPa/K)	σ_Y^M (MPa)
291.40	307.50	298	0.74	0.17	200
$\sigma_Y^{A,i}$ (MPa)	$\sigma_Y^{A,f}$ (MPa)	K_A (GPa)	K_M (GPa)	H_A (GPa)	H_M (GPa)
690	257.72	1.40	0.40	0.40	0.11

Moreover, the following parameters are calculated with the aid of Equations (33), (34), (37): $\varepsilon_R = 0.0033$, $T_C = 282.04$ K and $L = 9.18$ MPa/K.

At first, pseudoelastic effect is concerned regarding a SMA specimen subjected to an isothermal mechanical loading performed at $T = 333$ K ($T > T_A$). The stress–strain curve for stress driving cases is presented in Figure 4a. Notice that there are two different elastic moduli for the austenitic and martensitic phase. Figure 4b shows the volumetric fraction evolution of each phase, allowing the identification of phase transformation process. When the specimen is free of stress, the austenitic phase is stable. After this, positive stresses induce the formation of the $M+$ variant of martensite. The unloading process induces the austenite formation again. When there are negative stresses, the $M-$ variant of martensite is induced. Finally, the unloading process induces the formation of the austenitic phase (A).

The SME is now focused regarding a thermomechanical loading depicted in Figure 5a. Firstly, a constant temperature $T = 263$ K ($T < T_M$) is considered, where the martensitic phase is stable. After mechanical loading–unloading process, the specimen presents a residual strain that can be eliminated by a subsequent thermal loading (Figure 5a). Notice that the stress–strain–temperature curve represents the SME and it should be pointed out that there is a stable phase, associated with the twinned martensite (M), when the specimen is free of stress. The heating process induces the transformation from detwinned martensite, $M+$, to twinned martensite, M and, for higher temperatures, the austenitic phase (A). The nonlinear behavior promoted by phase transformation can be observed in the detailed zoom of Figure 5(a). Figure 5(b) shows the volumetric fraction evolution of each phase, pointing out the cited phase transformation.

The thermal expansion effect is now considered regarding a thermal loading depicted in Figure 6(a), free of stress. Figure 6(a) presents the strain–temperature curve, showing thermal expansion and phase transformations related to a thermal loading. Notice the hysteretic characteristics of phase transformation, defined by the critical temperature T_M (vertical line at 291.4 K). Experimental data presented by Jackson et al. (1972) show a similar curve, indicating that the model is

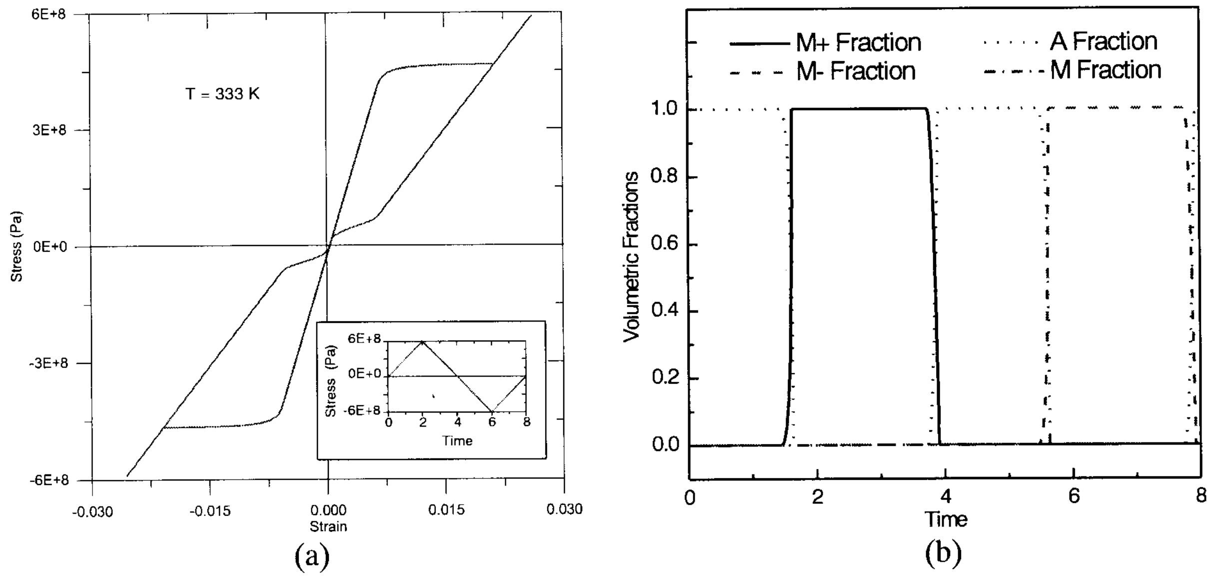


Figure 4. Pseudoelastic effect ($T = 333\,K > T_A$): (a) stress–strain curve; (b) volumetric fractions.

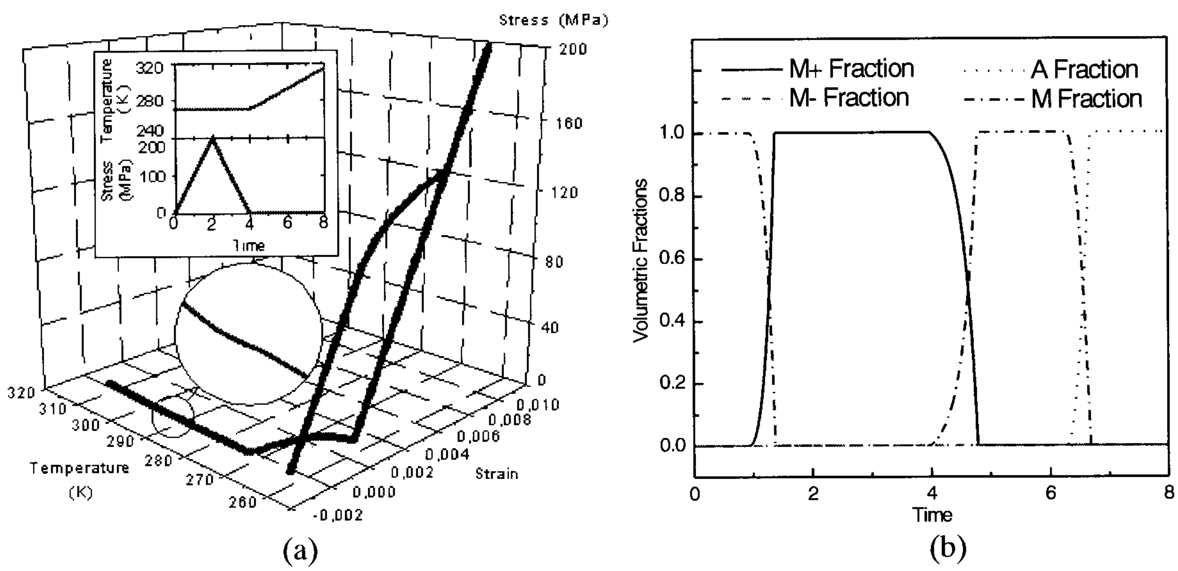
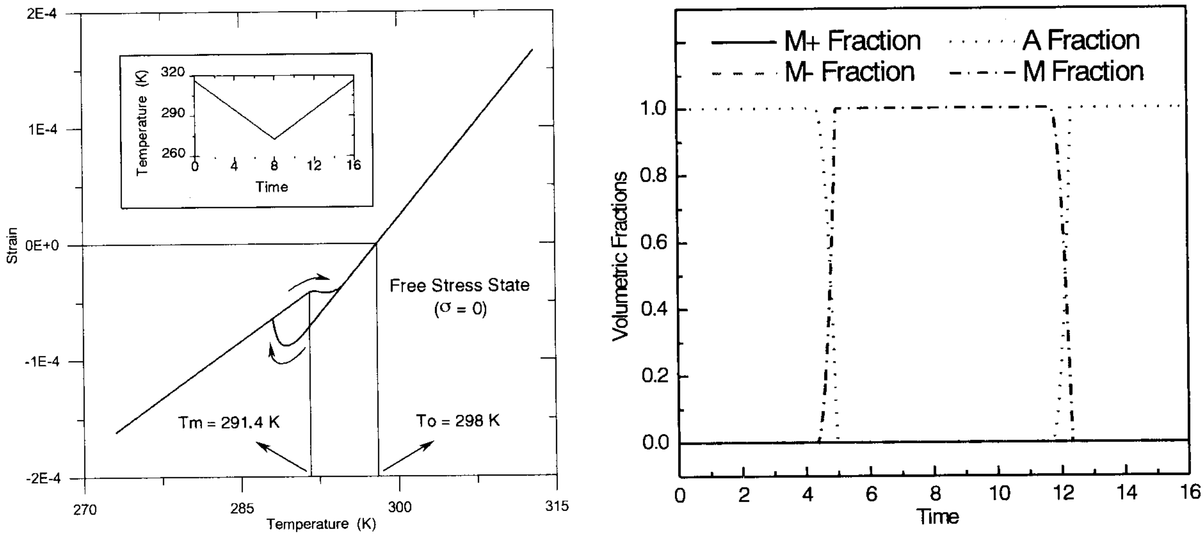


Figure 5. Shape memory effect ($T = 263\,K < T_M$): (a) stress–strain–temperature curve; (b) volumetric fractions.

capable to describe the coupling between SMEs and thermal expansion. Figure 6(b) presents the volumetric fraction evolution of each phase, showing the conversion between twinned martensite (M) and austenite (A).

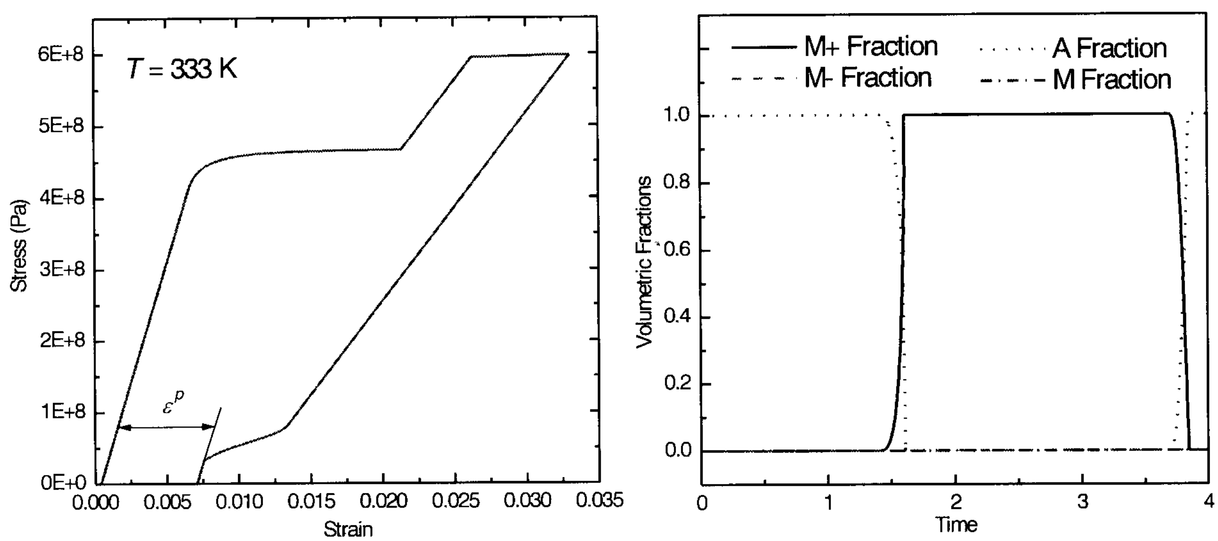
The forthcoming analysis concerns with the effect of plastic strains in the thermomechanical behavior of SMAs. The thermo-plastic parameter is $\eta_c = \eta_{ci} = \eta_{ck} = 0.02$. At first, an isothermal thermomechanical load is considered at $T = 333\,\text{K}$ ($T > T_A$), reaching the yield surface. Figure 7(a) shows stress–strain curve related to this loading–unloading process. During the loading process, after phase transformation ($A \rightarrow M+$), the yield limit is reached producing plastic strains. Upon unloading, reverse transformation ($M+ \rightarrow A$) is completed and SMA experiences a linear unloading. When the unloading process is finished, there are irreversible residual strains associated with plastification. The evolution of volumetric fractions shows the phase transformation related to these processes (Figure 7b).

At this point, a thermomechanical loading process is considered. Figure 8 presents the response of the SMA subjected to this process. Figure 8(a) shows a stress–strain curve. The loading process causes plastic strain after phase transformation is finished, when yield surface is reached. When mechanical loading–unloading process is finished, SMA presents residual strain.



(a) (b)

Figure 6. *Thermal expansion effect: (a) strain–temperature curve; (b) volumetric fractions.*



(a) (b)

Figure 7. *Pseudoelasticity with plastic strain: (a) stress–strain curve; (b) volumetric fraction.*

Heating the specimen can eliminate the reversible part of this residual strain, which is related to the phase transformation. Nevertheless, there are irreversible strains related to the plastification process. Figure 8(b) presents the evolution of volumetric fractions, showing phase transformation during loading–unloading process.

A nine-cycle thermomechanical loading process, depicted in Figure 9, is now considered. This process is a mechanical loading of the austenitic phase into the plastic region of strain followed by a temperature loading that promote phase transformation. Figure 10(a) presents stress–strain curves related to this loading process while Figure 10(b) shows the strain–temperature response. Figure 10(c) presents evolution of volumetric fractions. These results are in qualitative agreement with experimental data presented by Miller and Lagoudas (2000). Notice that the growth of plastic strains tends to change the phase transformation temperature and also to enlarge hysteresis loops. This behavior is related to the two-way SME.

Miller and Lagoudas (2000) use the term two-way strain to describe the strain that develops during the austenitic to martensitic phase transformation under zero load. This strain is the result of dislocation arrangements and typically, SMAs present positive two-way strains. In the cited reference, the authors

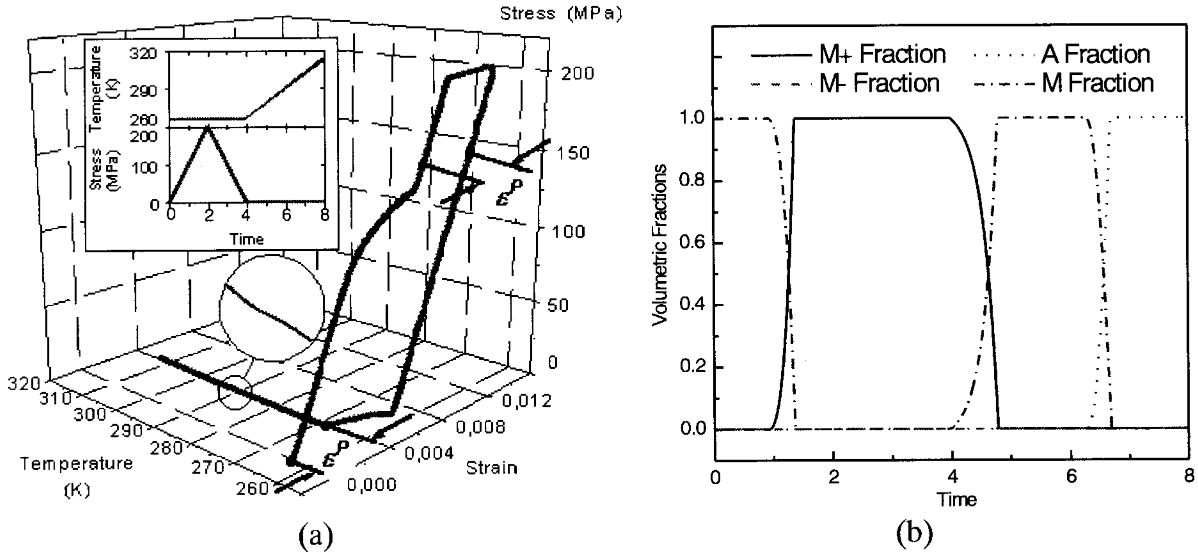


Figure 8. *Shape memory effect with plastic strains: (a) stress–strain curve; (b) volumetric fraction.*

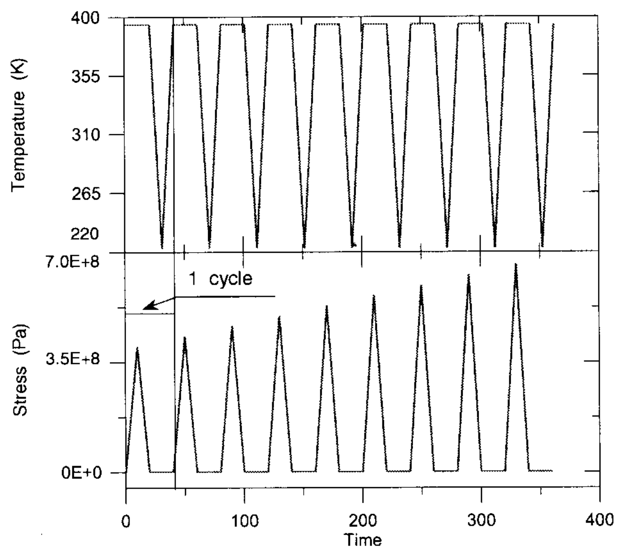


Figure 9. *Nine-cycle thermomechanical loading process.*

show experimental tests that present negative values for these strains. Miller and Lagoudas present an argument that this apparent discrepancy with theory may be explained by a previous heat treatment of the specimen. Figure 11 presents the first cycle of this nine-cycle test, showing that the argumentation of Miller and Lagoudas is correct. Since the temperature T_M may be altered by heat treatments (Tang and Sandström, 1995), it is possible to see how this alteration modifies the curves of phase transformation, changing the sign of two-way strain. Figure 11(a) considers $T_M = 291.4\,\text{K}$ while in Figure 11(b), $T_M = 307.5\,\text{K}$.

A discussion of the plastic-phase transformation coupling is now focused. With this aim, simulations with different values of the parameter η_c are performed. Figure 12 presents strain–temperature curves associated with the three first cycles of the previous test. Notice that plastic-phase transformation coupling parameter tends to change the phase transformation temperature, moving the hysteresis loop. This behavior is related to the growth of hysteresis loops.

The plastic-phase transformation coupling is now focused considering pseudoelastic and SMEs (Figure 13). The alteration of plastic-phase transformation coupling parameter, η_c, shows how this effect tends to anticipate phase transformation. It should be pointed out that this behavior could promote the loss of actuation of the SMA, since the anticipation of phase transformation reduces the amount of phase transformation deformation that can be recovered by either a thermal or a mechanical loading. Figure 13(a) shows pseudoelastic behavior for different values of coupling parameter. This variation can decrease the internal dissipation of SMA passive actuators, for example. On the other hand, Figure 13(b) shows a shape memory test, with constant temperature, where this behavior is illustrated. In this situation, the variation of coupling parameter can reduce either the deformation recovery or the force generated by a thermal actuation.

CONCLUSIONS

The present contribution proposes a 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, exhibits a stable phase when the material

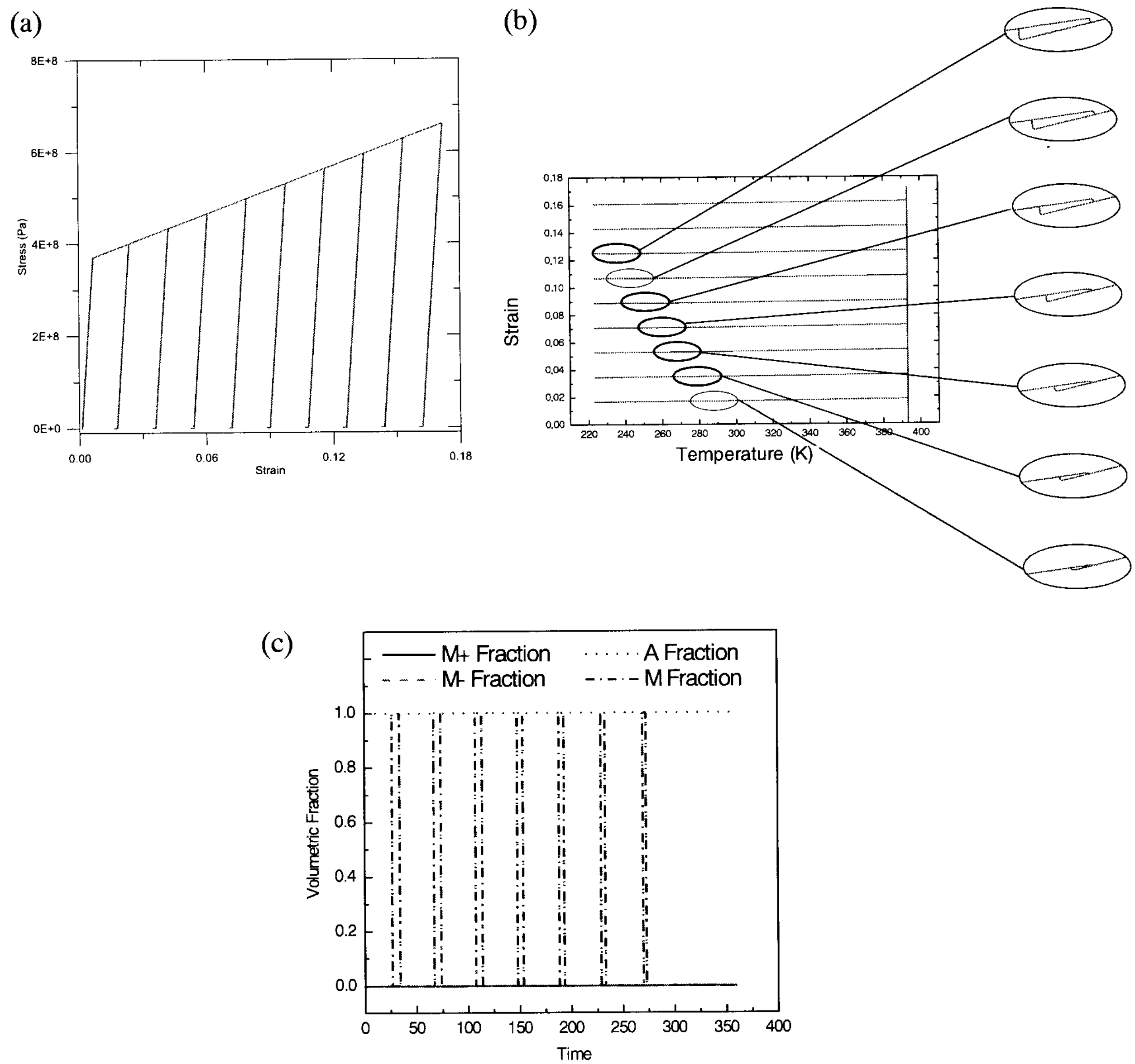


Figure 10. *Nine-cycle test: (a) stress–strain curve; (b) strain–temperature curve; (c) volumetric fractions.*

is free of stress at low temperatures. The consideration of different material parameters for austenite and martensite is another characteristic of the model. The inclusion of the constraint which establishes that the detwinned martensites does not exist in the absence of stresses, and also the thermal expansion term allows one to describe the phase transformation due to thermal expansion phenomena. Plastic strain description is another goal of the proposed model. Hardening effect is represented by a combination of linear kinematic and isotropic behaviors. A plastic-phase transformation coupling is incorporated into the model allowing a correct description of the thermomechanical behavior of SMAs. An iterative numerical procedure based on the operator split technique associated with an orthogonal projection and return mapping algorithms is developed. Numerical results show that the proposed model is capable to describe the main aspects of thermomechanical behavior of SMA. The plastic-phase transformation coupling allows the description of the two-way SME. Furthermore, this coupling tends to anticipate phase transformation, also changing its temperature, after plastic strains occur. Even though results predicted by the proposed model present qualitative agreement with experiments, some improvements are necessary in order to obtain closer quantitative agreement. Furthermore, there are features that still needed to be contemplated in the proposed model. The elimination of the softening behavior for strain driving case and the correct description of internal loops observed during cyclic loads associated with incomplete phase transformations are some examples.

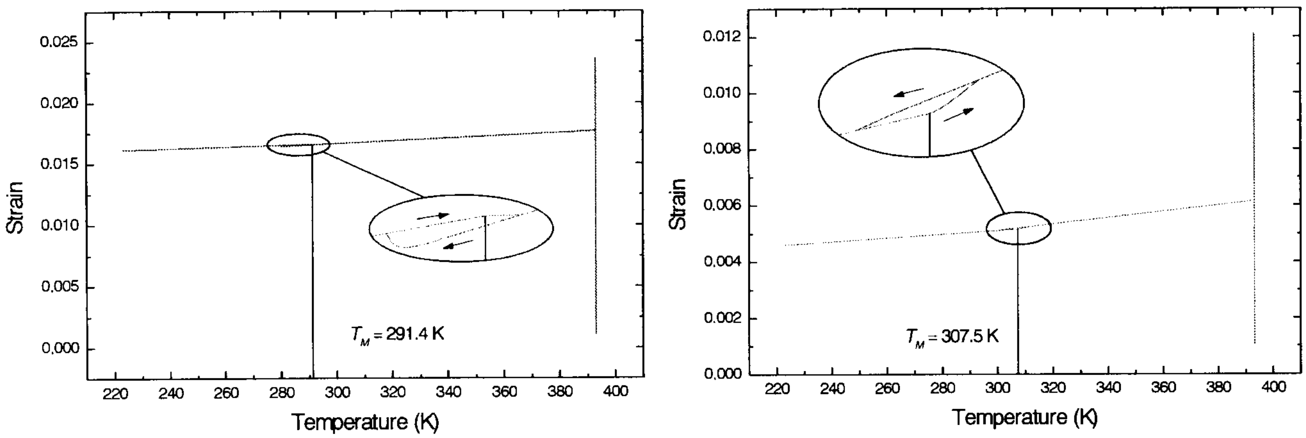


Figure 11. *One cycle of the nine-cycle test: strain–temperature curve: (a) $T_M = 291.4$ K; (b) $T_M = 307.5$ K.*

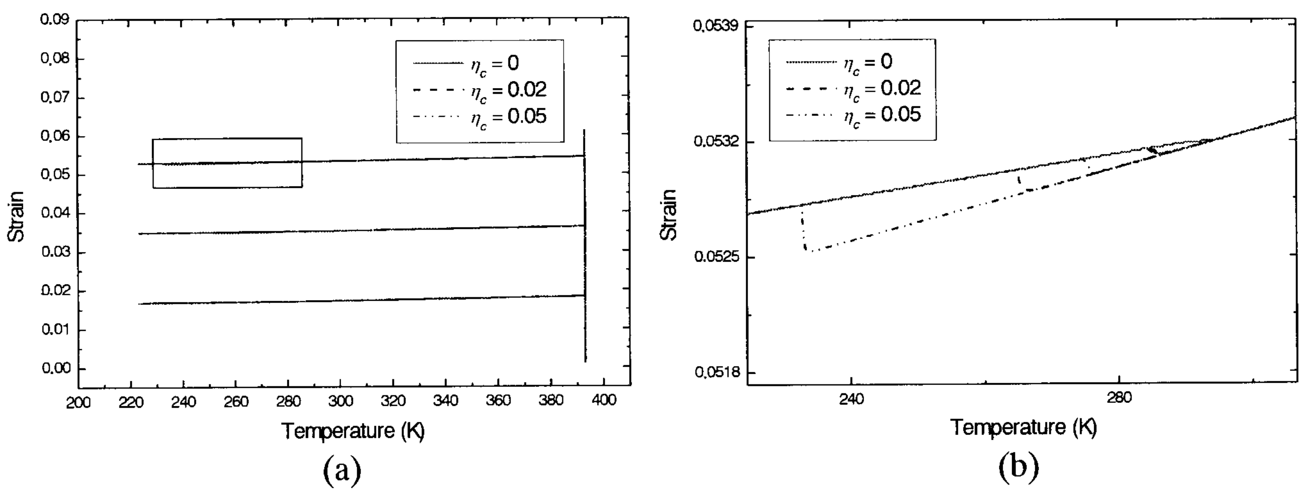


Figure 12. *Effect of plastic-phase transformation coupling: strain–temperature curves: (a) three cycles; (b) enlargement.*

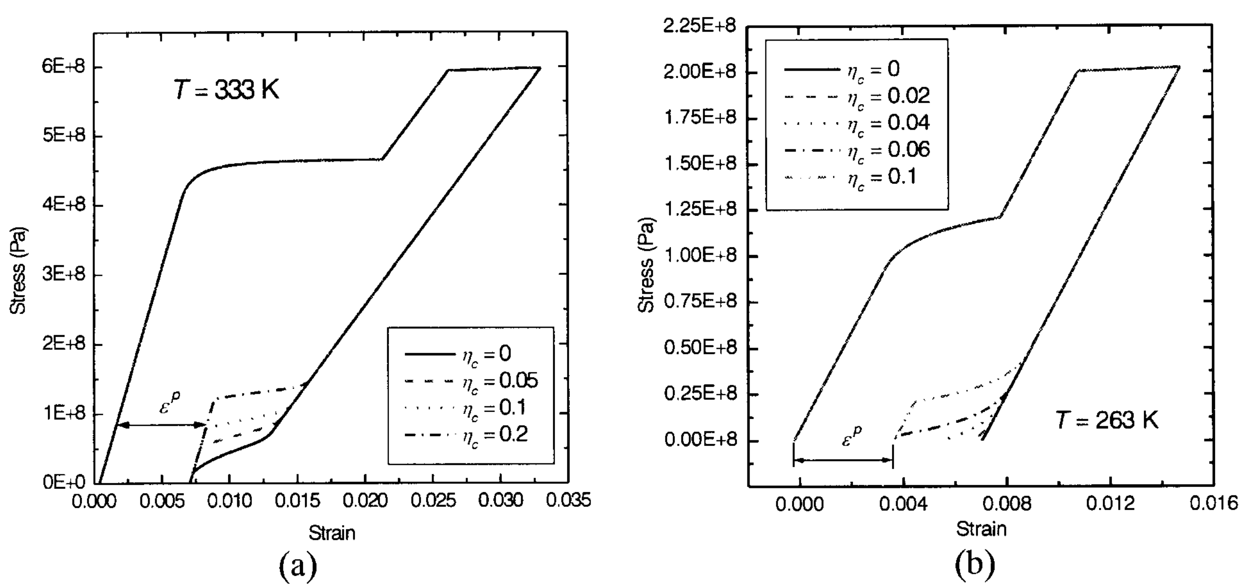


Figure 13. *Effect of plastic-phase transformation coupling: stress–strain curves: (a) pseudoelasticity; (b) shape memory.*

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