Title

A Uniaxial Model for Shape-Memory Alloys

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Abstract

The purpose of this work is to present a uniaxial model for shape memory alloys, cast within the framework of a previously developed theory of inelastic behavior that is general and flexible. The model is based on a single internal variable (the martensite fraction), for which an evolution equation in rate form is proposed. The response of the model under cyclic stress and/or thermal paths is presented and discussed. Despite its simplicity, the model is able to predict the shape-memory effect and pseudoelastic behavior; moreover, for loading-unloading cycles, without completion of the phase transition, the model has a cyclic response with internal loops.

1 Introduction

Materials undergoing solid-solid phase transitions are receiving increased attention, mainly for their innovative use in practical applications. Within this large class of materials, an important place is occupied by *shape-memory alloys* (SMAs) (Duerig 1990).

Under stress and/or thermal loading, an SMA presents a peculiar response behavior, due to a *martensitic transformation* between a more ordered phase, called *parent phase* or *austenite*, and a less ordered phase, called *martensite*. This solid-solid phase transformation gives the material an intrinsic capacity to *remember* its initial shape. Due to the interaction between several different effects at the microlevel, the development of macroconstitutive models based on the micromechanics of the phase transition is a sophisticated and difficult task. Consequently, there have been several attempts to construct phenomenological models capable of representing the SMA macrobehavior. Representative works are by: Abeyaratne and Knowles (1993), Brandon and Rogers (1992) Brinson (1993), Cory and McNichols Jr. (1985, 1987), Falk and Konopka (1990), Ivshin and Pence (1993a, 1993b), Liang and Rogers (1990, 1992), Muller and Xu (1991), Patoor, Eberhardt and Berveiller (1988), Tanaka et al. (1982, 1985, 1986, 1992), Tobushi et al. (1991), Wilmanski (1993).

In the present work we propose a new phenomenological model, developed within the framework of the *theory for continua undergoing phase transitions* presented by the authors in Reference (Auricchio 1993). The model is based on a single internal variable (the martensite fraction) for which an evolution equation in rate form is presented. The characteristics of the model that make it particularly appealing are:

- simplicity,
- complete soundness in a valid continuum-mechanics framework,
- possibility of extending the model to describe more complex behavior,
- possibility of extending the model to a general three-dimensional theory,
- possibility to numerically implement the model (or its generalization) in a valid computational framework (such as finite elements).

The paper is organized as follows: in Section 2 we briefly review the shape-memory alloy macroresponse, pointing out the complexity of the micromechanics involved. In Section 3 we present the new model and in Section 4 we test it under different cyclic loading paths.

2 Micro- and macromechanics of shape-memory alloys

The term *shape-memory alloy* is usually adopted for materials which show an intrinsic capacity of remembering their original configuration or shape [1]. From a macroresponse point of view (that is, in terms of macroscopic response quantities, such as stress, strain and temperature) shape-memory alloys present two main properties: *shape-memory effect* (SME) and *pseudoelasticity* (PE). In what follows we briefly describe the meaning of this terminology:

- **Shape-memory effect (SME).** Consider a specimen in the austenitic state and at a temperature, characteristic of the specific alloy, such that at zero stress both austenite and martensite are stable. Let the specimen now be deformed so as to induce large inelastic strains, due to a stress-induced conversion of austenite into martensite. The inelastic strains may be completely recovered if the material is heated, causing a temperature-induced inverse transformation (conversion of martensite into austenite). Figure 1 gives a graphic description of the process.

- **Pseudoelasticity (PE).** Consider a specimen in the austenitic state and at a temperature, characteristic of the specific alloy, such that at zero stress only the austenite is stable. If the specimen is deformed, the material usually presents a highly nonlinear behavior, due to a stress-induced conversion of austenite into martenste. However, when unloading occurs, a reverse transformation (from martensite to austenite) occurs, as a result of the instability of the martensite at zero stress

[1] In the literature it is possible to find many introductory papers describing shape-memory alloys, such as those by Wayman (1992, 1993), Wayman and Duerig (1990). Refer to these for a more detailed, but still introductory, presentation on such materials.

and at the given temperature, such that at the end no residual permanent strains are present [2]. The stress-strain path described during the loading-unloading process usually presents a hysteresis loop, as qualitatively presented in Figure 2.

Both effects are strictly related to a martensitic transformation. From the metallurgic point of view (Khachaturyan 1983, Wayman 1964), a martensitic transformation is a solid-solid, diffusionless, crystallographicly reversible transition between a more ordered phase, called the *parent phase* or *austenite*, and a less ordered phase, called *martensite*. For the case of SMAs the transformation is also rate-independent. However, the resulting macroscopic bahavior is not simply the result of the martensitic transformation, since several other mechanisms play an important role and moreover interact with one another (Funakubo 1987, Otsuka 1986). As examples, we may consider NiTi (Nitinol), described in References (Funakubo 1987, Curtis 1972, Melton 1990). . From a crystallographic point of view the phase transformation is associated with a cubic-to-monoclinic change of crystal symmetry. However, the presence of monoclinic martensite in a cubic austenitic matrix as well as the fact that the martensite grows as plate-like inclusions in the matrix generate misfit problems; accordingly, macro-twinned and micro-twninned structures are formed to accomodate all the different misfits.

From the previous discussion it is clear that it is difficult to develop a continuum-mechanics model, starting from the basic micromechanics of the transformation. On the other hand, SMA-based devices are currently constructed and used (Duerig 1990); consequently, in order to design of such devices in a safe, functional and correct manner, a capacity of simulating material behavior under very specific and sometimes complex loading patterns is required. Being aware of this need, in what follows we present a phenomenological constitutive model which reproduces the basic features of shape-memory alloy macroresponse.

Though the model is presented in a uniaxial context, it may be extended to the three-dimensional case, since it is cast in a correct continuum-mechanics theory. Such an extension, and the relative implementation in a real computational and design environment (such as a finite-element code)

[2]Some papers prefer to use the term *superelasticity* for this phenomenon, distinguishing between so-called *rubberlike* behavior and superelasticity, and using the term *pseudoelasticity* for both.

will be discussed in forthcoming papers.

3 A uniaxial model for shape-memory alloys

The general and flexible inelastic theory described in Reference (Auricchio93) is a convenient framework for the development of constitutive equations for materials in which phase transitions may occur. In accordance with this theory, we need to specify:

- state and internal variables,
- transition zones and rules for the activations of the phase transitions.

In what follows we describe the corresponding choices as the basis of the model developed here.

Control and internal variables. As control variables we assume the uniaxial stress σ and the temperature T. As the internal variable, the most natural candidate is the *martensite fraction* ξ_M. By convention, $\xi_M = 0$ means no martensite, hence the material is completely in the austenitic phase, while $\xi_M = 1$ means that the material is completely in the martensitic phase. Similarly, we may also introduce the *austenite fraction* ξ_A. The two parameters, ξ_M and ξ_A, are clearly not independent, and the following relation (viewed as a constraint!) must be fulfilled at any time:

$$\xi_M + \xi_A = 1 \tag{3.1}$$

Accordingly:

$$\dot{\xi}_M + \dot{\xi}_A = 0 \tag{3.2}$$

where a superposed dot indicates the time derivative. In what follows, we initially choose to work with both fractions, since it simplifies the development of the model. However, due to equation 3.1, the model has only one independent internal variable and, accordingly, at the end of the section we express the whole model only in terms of the martensite fraction [3].

Transition zones and activation rules. The SMA presents two solid-solid phase transformations:

[3]Note that we restrict the discussion to the case of only one scalar internal variable; however, to describe more complex phenomenologies, the model may be extended and should include more internal variables.

- production of martensite, which means conversion of austenite into martensite ($A \rightarrow M$),
- production of austenite, which means conversion of martensite into austenite ($M \rightarrow A$)

Experimentally it has been shown that in a stress-temperature diagram and in the usual range of applications, each region may be assumed to be delimited by two parallel straight lines (Funakubo 1987). Let now discuss the two processes in more detail.

- *PRODUCTION OF MARTENSITE.* As represented in Figure 3, the straight lines which delimit the transition zone for the production of martensite are:

$$\begin{aligned} F_1 &= \sigma - C_M(T - M_s) \\ F_2 &= \sigma - C_M(T - M_f) \end{aligned}$$

where C_M is a material parameter, and M_s and M_f are the starting and final temperatures at which the transformation may occur at zero stress. Accordingly, the region in which the transformation may take place is described by:

$$F_1 > 0 \ , \ F_2 < 0 \quad \Rightarrow \quad F_1 F_2 < 0$$

Moreover, recalling the physics of the problem, we note that the conditions for the production of martensite are a stress increase, a temperature decrease or a combined action; such conditions may condensed in the form:

$$\dot{F}_1 > 0$$

Hence, the rate of martensite production must be of the form:

$$\dot{\xi}_M = K_M < -F_1 F_2 >< \dot{F}_1 > \tag{3.3}$$

where K_M is a scalar function of the state variable (control and internal variables), and $< . >$ is the Macaulay bracket defined by $< x >= 1/2(x + |x|)$. For now, we leave K_M unspecified.

- *PRODUCTION OF AUSTENITE.* As represented in Figure 4, the straight lines which delimit the transition zone for the production of martensite are:

$$\begin{aligned} F_3 &= \sigma - C_A(T - A_s) \\ F_4 &= \sigma - C_A(T - A_f) \end{aligned}$$

where: C_A is a material parameter, A_s and A_f are the starting and the final temperature at which the transformation may occur at zero stress. Accordingly, the region in which the transformation may take place is described by:

$$F_3 < 0 \ , \ F_4 > 0 \quad \Rightarrow \quad F_3 F_4 < 0$$

Again we note that the conditions for the production of austenite are a stress decrease, a temperature increase or a combined action; such condition may be condensed in the form:

$$\dot{F}_3 < 0$$

Hence, the rate of austenite production (the opposite of the martensite production) must be of the form:

$$\dot{\xi}_A = K_A < -F_3 F_4 >< -\dot{F}_3 > \tag{3.4}$$

where K_A is another scalar function of the state variables left unspecified for now.

We wish to stress that, because of the general framework in which the model is developed (i.e. the inelastic theory described in Reference [Auricchio 1993]), there is no limitation on the relative position of the two phase-transition zones; hence they may intersect or they may be disjoint, since neither case would be critical for the constitutive model developed in the present paper.

We are now left only with choosing a specific form for K_M and K_A to give specific form to the flow rules. In the following discussion, we restrict our attention to the following simple forms:

$$\dot{\xi}_M = \beta_M(1-\xi_M)\ \frac{<-F_1F_2>}{|F_1F_2|}\ \frac{<\dot{F}_1>}{(F_2)^2} \qquad A \rightarrow M$$
$$\dot{\xi}_A = \beta_A(1-\xi_A)\ \frac{<-F_3F_4>}{|F_3F_4|}\ \frac{<-\dot{F}_3>}{(F_4)^2} \qquad M \rightarrow A$$

where β_M and β_A are two scalar constants, measuring the respective rates at which the $A \rightarrow M$ and the $M \rightarrow A$ transformations proceed. Clearly, other choices of K_M and K_A are possible.

Recalling equations 3.1 and 3.2, we may now express the production of austenite ($M \rightarrow A$) in terms of ξ_M and $\dot{\xi}_M$, i.e. as reduction of martensite:

$$\dot{\xi}_M = -\beta_A\xi_M \frac{<-F_3F_4>}{|F_3F_4|}\frac{<-\dot{F}_3>}{(F_4)^2} \qquad M \rightarrow A$$

Since the Macaulay brackets manage the choice of the active evolution process, we may sum the two evolutionary equations, obtaining a unique rule for the material:

$$\begin{aligned} \dot{\xi}_M &= (1-\xi_M)\beta_M\ \frac{<-F_1F_2>}{|F_1F_2|}\ \frac{<\dot{F}_1>}{(F_2)^2} \\ &\quad -\xi_M\beta_A\ \frac{<-F_3F_4>}{|F_3F_4|}\ \frac{<-\dot{F}_3>}{(F_4)^2} \end{aligned} \tag{3.5}$$

Note that due the simple form chosen for the K_M and K_A functions, the flow rule may be integrated in closed form and used to solve problems analytically.

Finally, for the constitutive equation for the stress we choose a linear dependence on the strain, the martensite fraction and the temperature variation. Accordingly:

$$\sigma = D\,(\epsilon - \epsilon_L\xi_M) - \alpha(T - T_0) \tag{3.6}$$

where D is the elastic modulus, ϵ is the total uniaxial strain, ϵ_L is the maximum residual strain (regarded as a material constant), ξ_M is the martensite fraction, α is the coefficient of thermal expansion, T is the temperature of the specimen, and T_0 is a reference temperature at which the specimen is unstressed.

4 Numerical examples

In what follows we present some applications of the theory developed so far. The material parameters chosen for the analysis are:

$$D = 10 \qquad C_M = C_A = 1 \qquad \epsilon_L = 10 \qquad T_0 = 50$$
$$\alpha = 10 \qquad M_f = 5 \qquad M_s = 40 \qquad A_s = 60 \qquad A_f = 90$$

The β-parameters, which measure the rate of the evolution processes, are always set equal to 1, unless explicitly stated otherwise. The material is assumed to start from a fully austenitic phase ($\xi_M = 0$).

For each analysis we first plot the control variables (stress and temperature) versus time; we then present the evolution in time of the martensite fraction (ξ_M, *xi_m* in the plots) and strain, as well as the relations between stress and strain and between temperature and strain. We believe that a complete understanding of the model behavior can be gained from these results.

In the following we briefly describe the examples presented and discuss the results obtained.

4.1 Single stress cycle at constant temperature.

We simulate the path graphically presented in Figure 5, which is a stress cycle at constant temperature ($T = 100 > A_f = 90$). The specimen is first loaded to have a complete stress-induced transformation (from austenite to martensite); upon unloading, a complete reverse transformation occurs (from martensite to austenite), since martensite is unstable at temperatures greater than A_f and zero stress (Figure 6). The analysis shows that the model predicts the pseudoelastic behavior described in Section 2 and qualitatively presented in Figure 2.

4.2 Single temperature cycle at constant stress.

We simulate the path graphically presented in Figure 7, which is a temperature cycle at constant (zero) stress. Starting at a temperature $T = 100$ ($T > A_f = 90$), the specimen is initially cooled, causing a complete temperature-induced transformation (from austenite to martensite); the specimen is then heated, causing the reverse transformation (from martensite to austenite).

The results of the analysis are presented in Figure 8. Note that the temperature-strain diagram also presents a hysteretic path.

4.3 Multiple stress cycles at constant temperature.

We test the behavior of the model under multiple stress cycles, while keeping the temperature constant (Figure 5). In particular, we consider the following three cases:

- partial reloading
- partial unloading
- partial unloading-reloading

where *partial reloading* implies an incomplete direct transformation (from austenite to martensite), while *partial unloading* implies an incomplete reverse transformation (from martensite to austenite). The results are presented in Figures 9, 10 and 11, and for each case the model presents the appropriate qualitative behavior, as experimentally described in several sources, such as References (Mcnichols 1987, Muller 1991). For the case of partial unloading-reloading (Figure 11) the stress-strain curve describes a series of loops, which are internal to the complete loading-unloading cycle; in particular the internal loops present ratcheting, which stabilize after a few cycles.

4.4 Combined stress-temperature cycle.

We simulate the path graphically presented in Figure 12, which is a stress cycle (path 1-2-3 in Figure 12) followed by a thermal cycle (path 3-4-5). The initial temperature is $T = 50$ ($M_s = 40 < T < A_f = 90$). The result of the analysis are presented in Figure 13. At the end of the stress cycle the material is completely in the martensitic state (since $T < A_f$, the martensite is stable at zero stress) and accordingly shows some permanent deformation (clearly indicated by the non-zero strain value at time 2). However, this permanent deformation is recovered after the thermal cycle; in the course of heating, the martensite is completely transformed into austenite. This analysis shows that the model can predict the shape-memory behavior described in Section 2 and qualitatively presented in Figure 1.

4.5 Test of rate parameters.

With this final analysis, we test the influence of the β-parameters in the model, i.e. β_M and β_A. We run a single stress cycle at constant temperature (as in Section 4.1), choosing $\beta_M = \beta_A = 50$, which is a value much larger than the one used in the first analysis presented. If the results presented in Figure 6 are compared with those presented in Figure 14 (for example in terms of evolution of martensite fraction or stress-strain curve), one may conclude that larger values of the β-parameters correspond to slower transformations.

5 Closure and future directions of research

In the present work we have presented a uniaxial model for shape-memory alloys, cast within the framework of a general and flexible inelastic theory that was previously developed (Auricchio 1993). The model is based on a single internal variable (the martensite fraction), for which an evolution equation in rate form is presented. The response of the model under cyclic stress and/or thermal paths is presented and discussed. Despite its simplicity, the model can predict the shape-memory effect and the pseudoelastic behavior; moreover, for loading-unloading cycles, without completion of the phase transition, the model shows a cyclic response with internal loops.

Though the model is developed in a uniaxial context, it may be extended to the three-dimensional case and to describe more complex behaviors, since it is cast in a consistent continuum-mechanics framework. Such extensions, and their corresponding implementation in a real computational and design environment, such as a finite-element code, will be presented in forthcoming papers.

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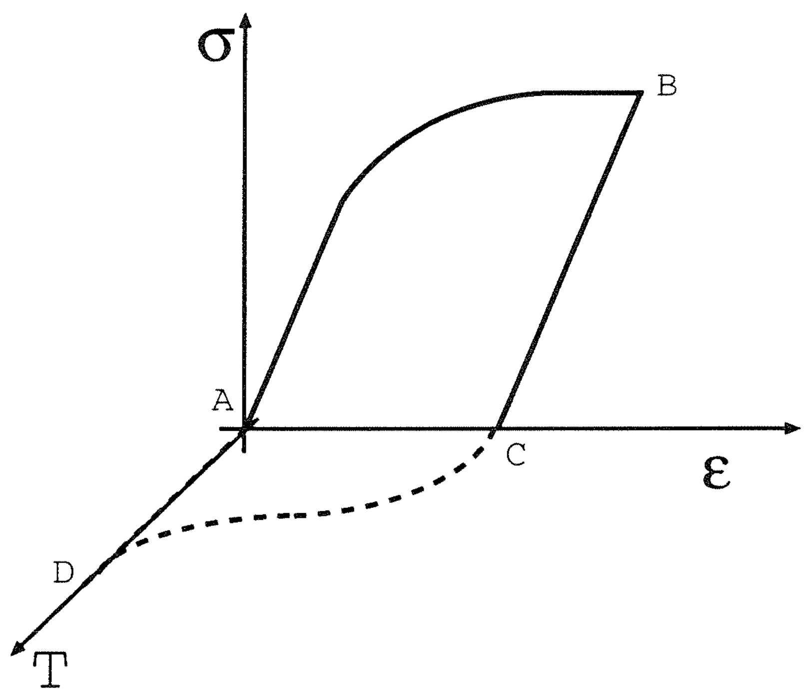

Figure 1: Shape memory effect. The continuous line is due to a stress loading path (AB), followed by unloading (BC), at the end of which the material presents permanent deformation (AC). The permanent strain may be recovered upon heating the material (CDA), represented with a dotted line.

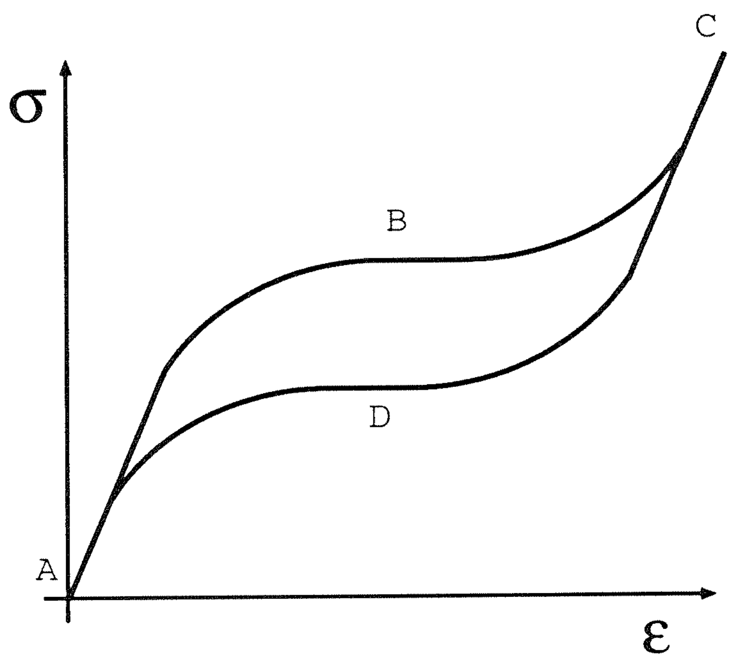

Figure 2: Pseudo-elasticity. At constant temperature the material is first loaded (ABC), showing a nonlinear behavior due to an $A \rightarrow M$ transformation. When unloaded (CDA), the reverse transformation $M \rightarrow A$ occurs, with zero final permanent strain. Note the hysteretic path.

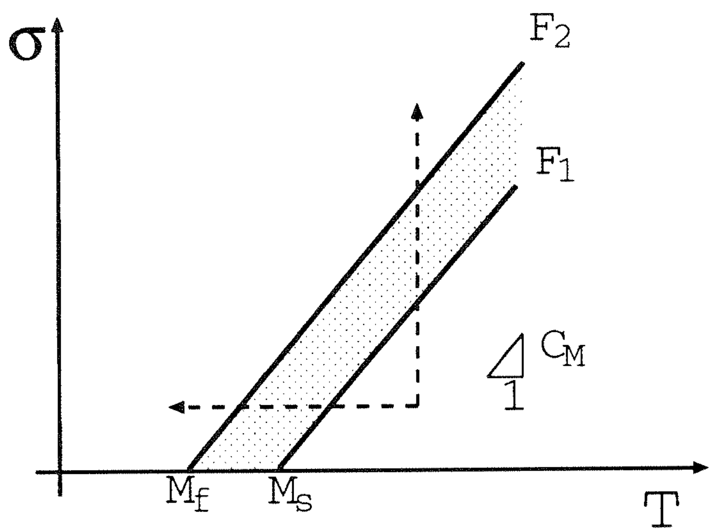

Figure 3: Production of martensite. Transition zone and directions of activation.

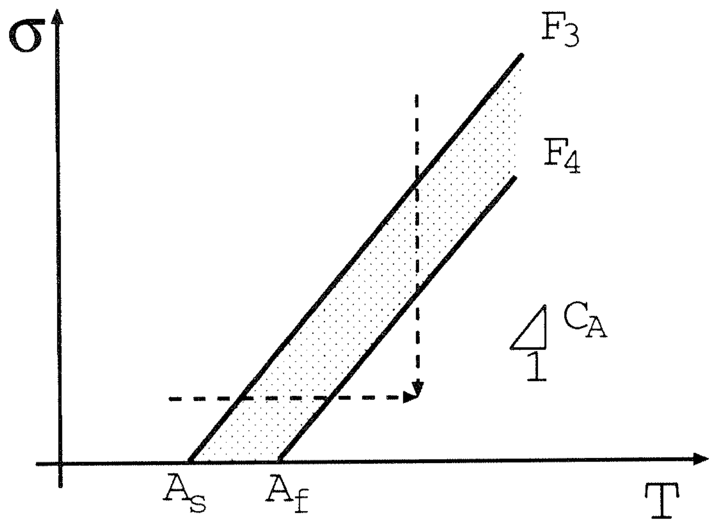

Figure 4: Production of austenite. Transition zone and directions of activation.

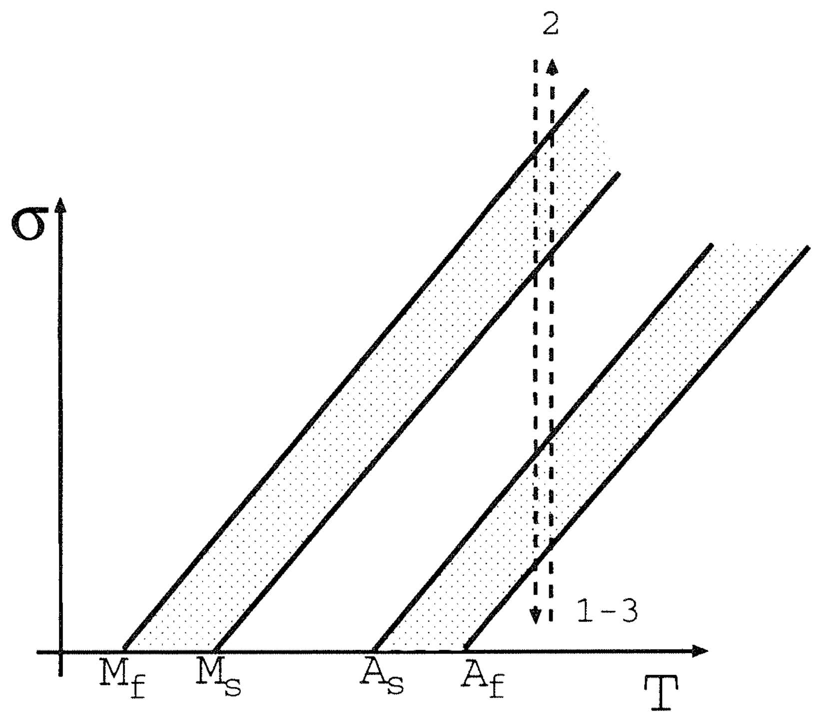

Figure 5: Stress cycle at constant temperature: path in the $T - \sigma$ plane.

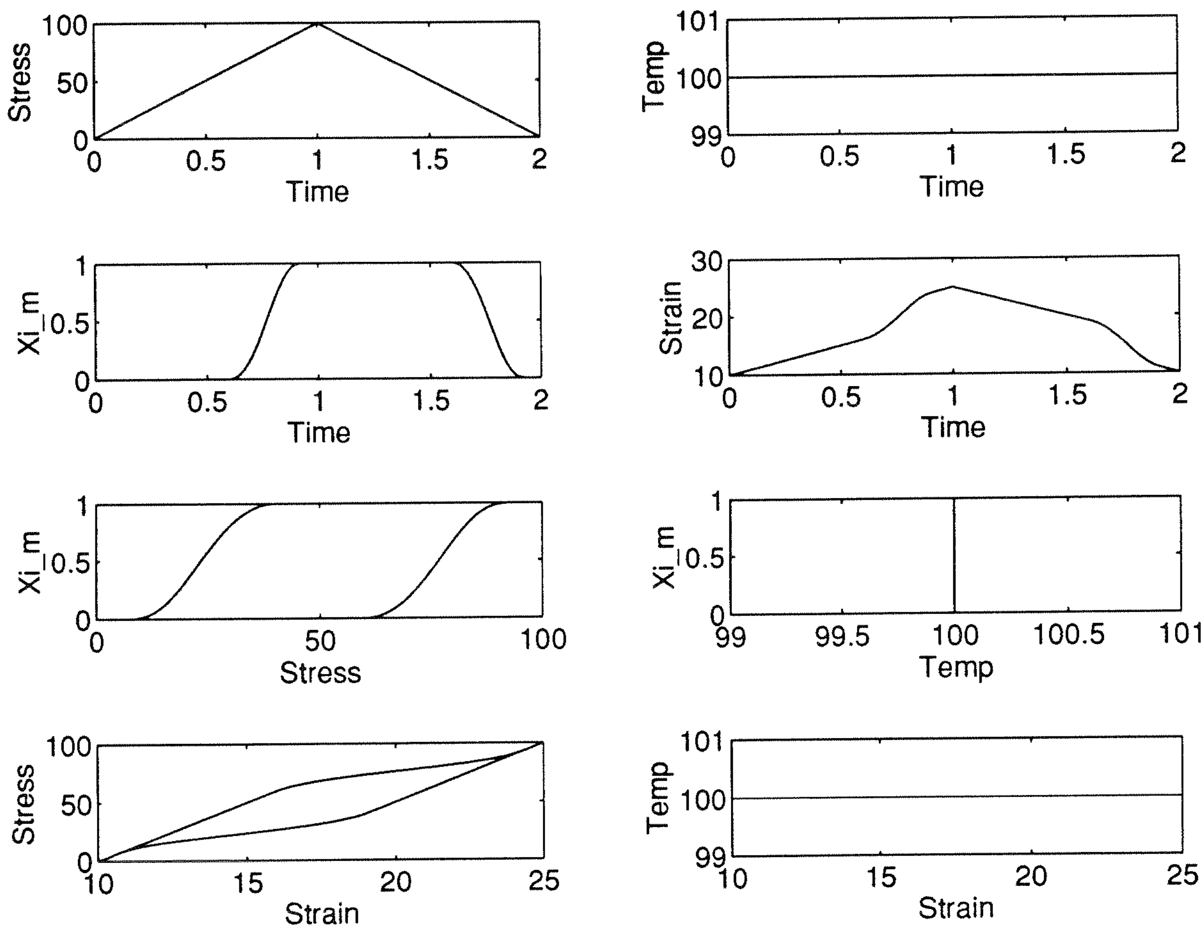

Figure 6: Stress cycle at constant temperature: response of the model.

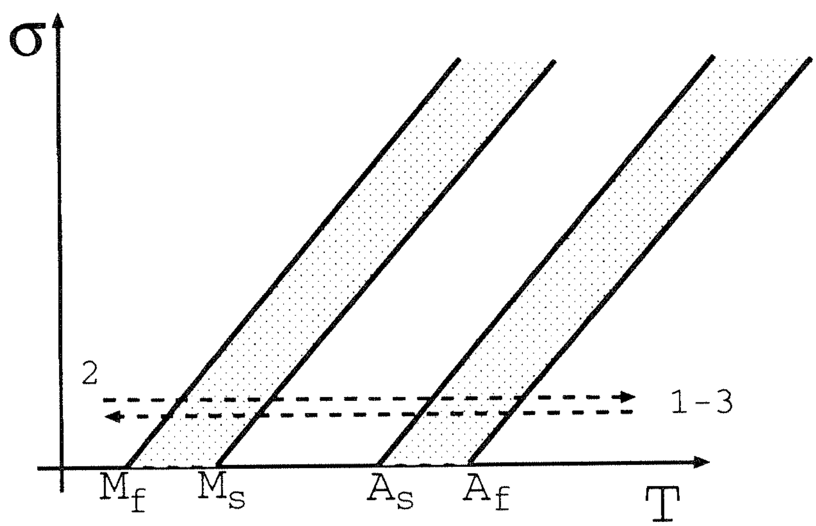

Figure 7: Temperature cycle at constant stress: path in the $T - \sigma$ plane.

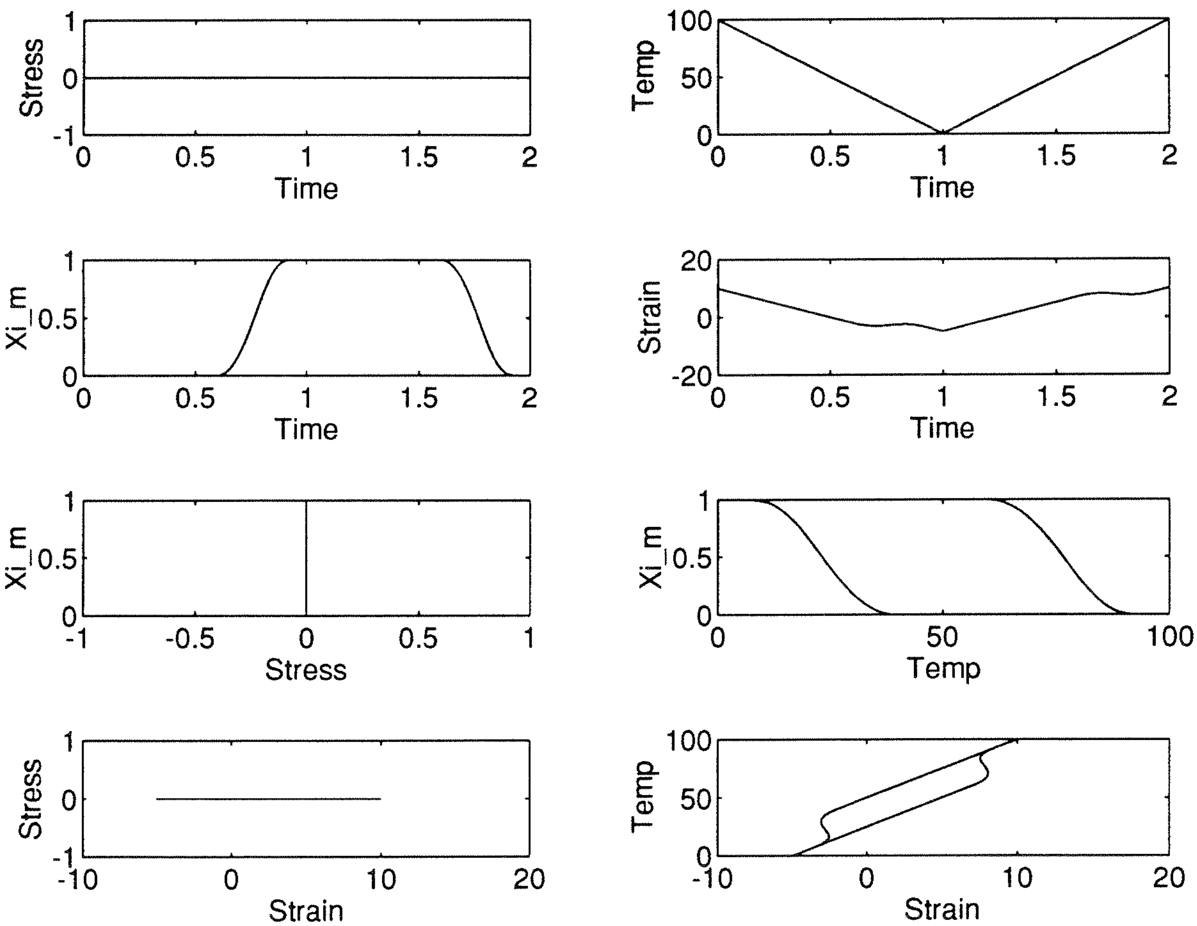

Figure 8: Temperature cycle at constant stress: response of the model.

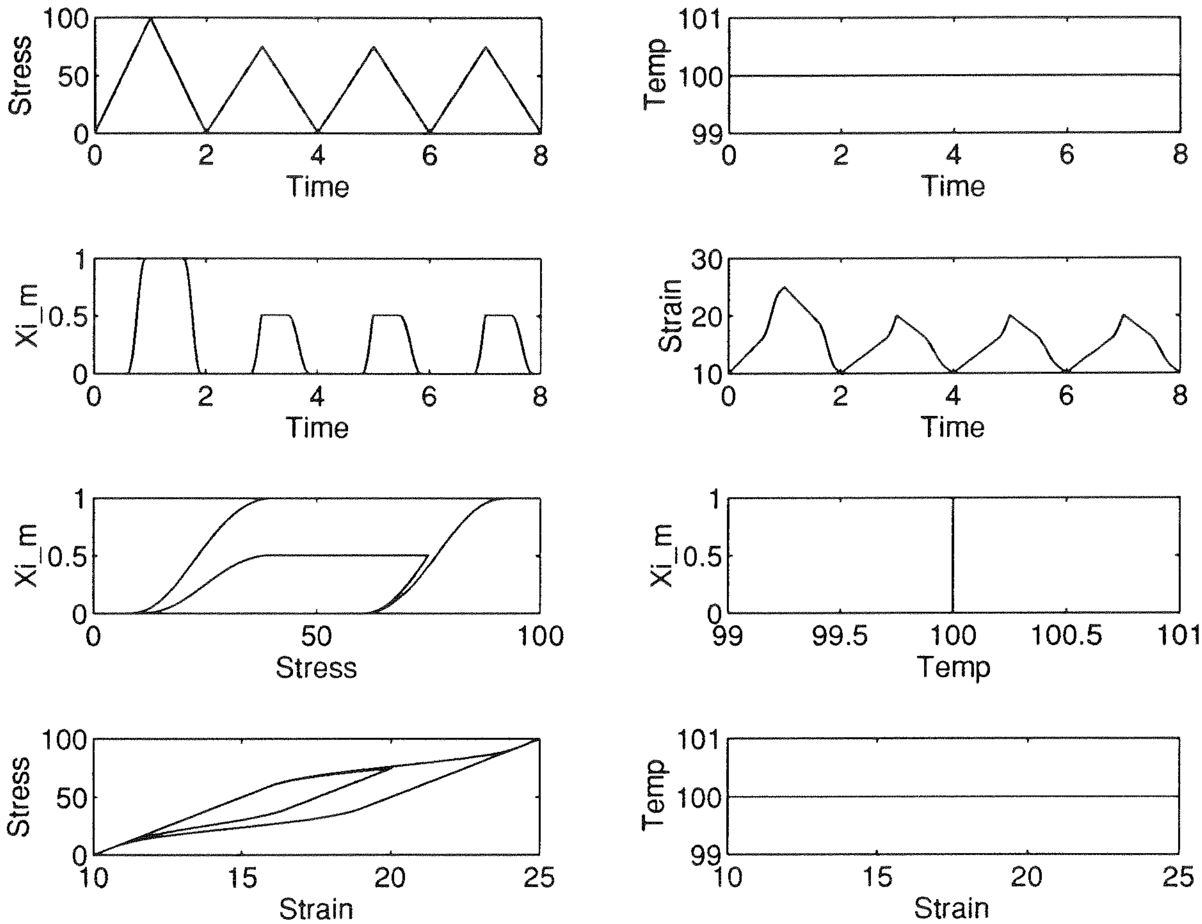

Figure 9: Stress cycles at constant temperature: response of the model under partial reloading.

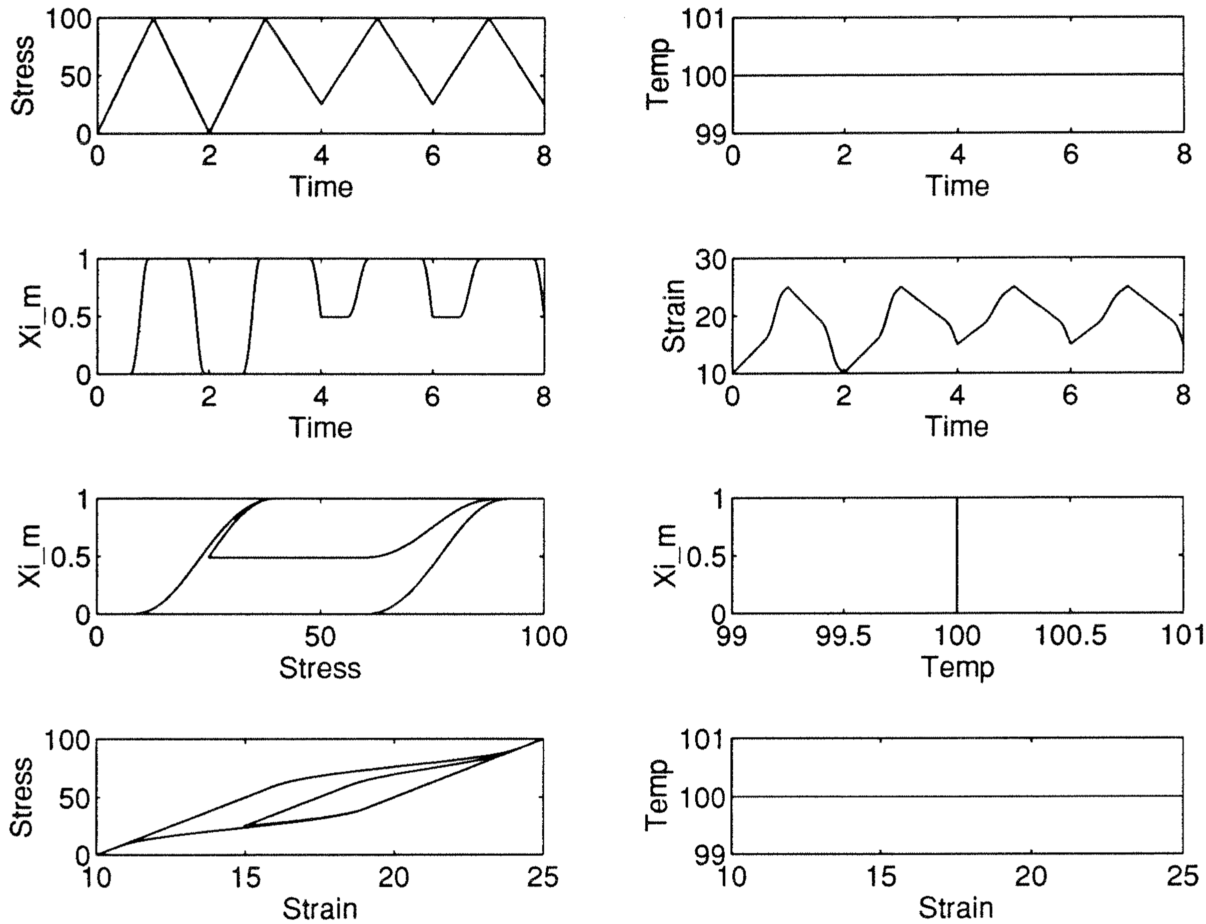

Figure 10: Stress cycles at constant temperature: response of the model under partial unloading.

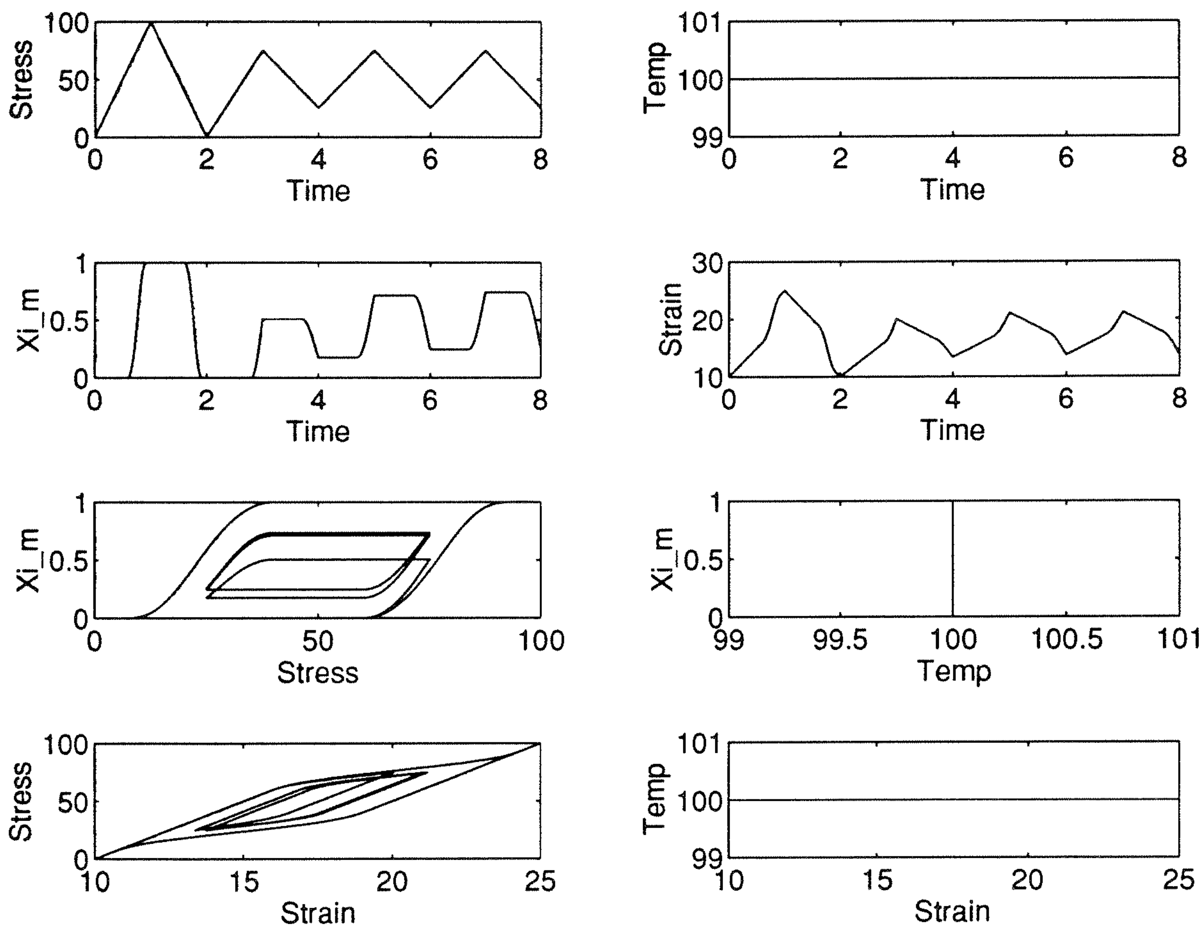

Figure 11: Stress cycles at constant temperature: response of the model under partial unloading-reloading.

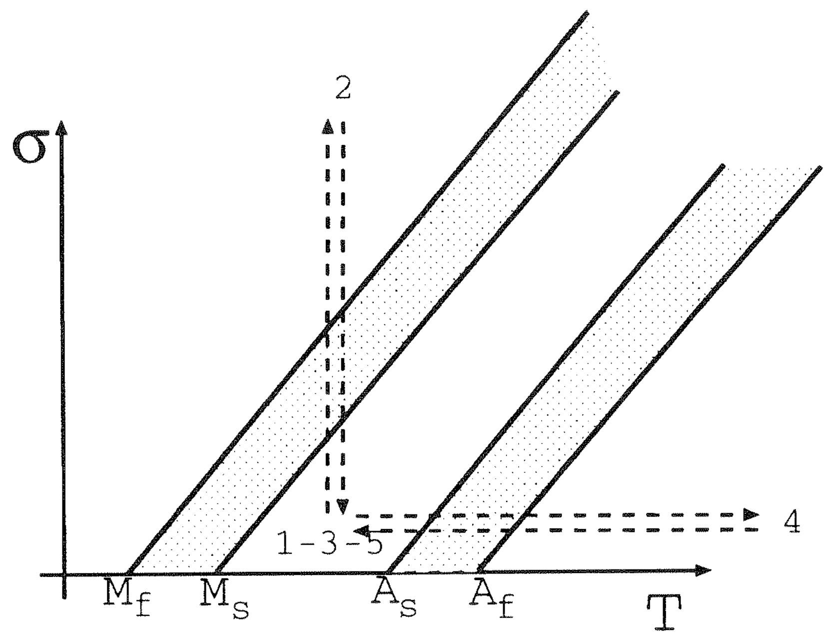

Figure 12: Combined stress-temperature cycles: shape-memory effect test.

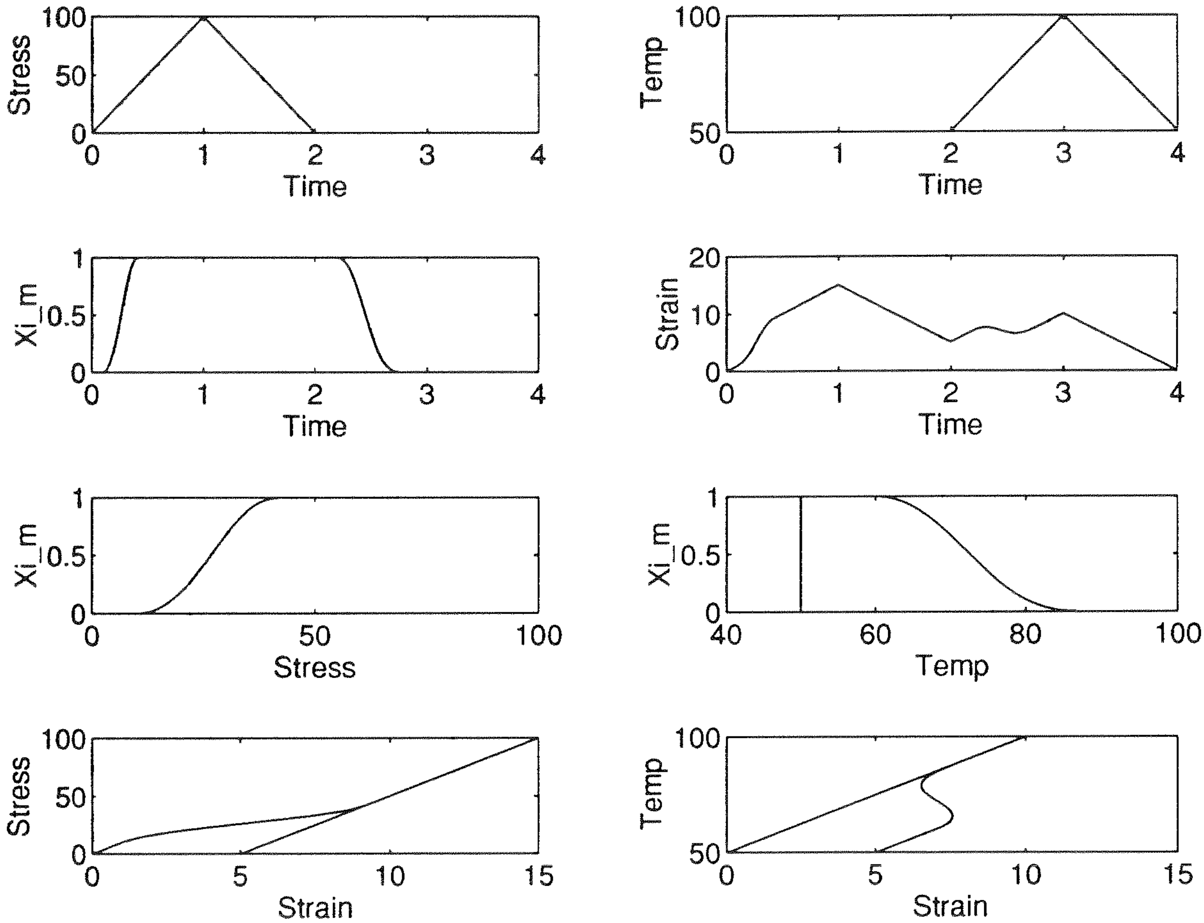

Figure 13: Combined stress-temperature cycles: response of the model.

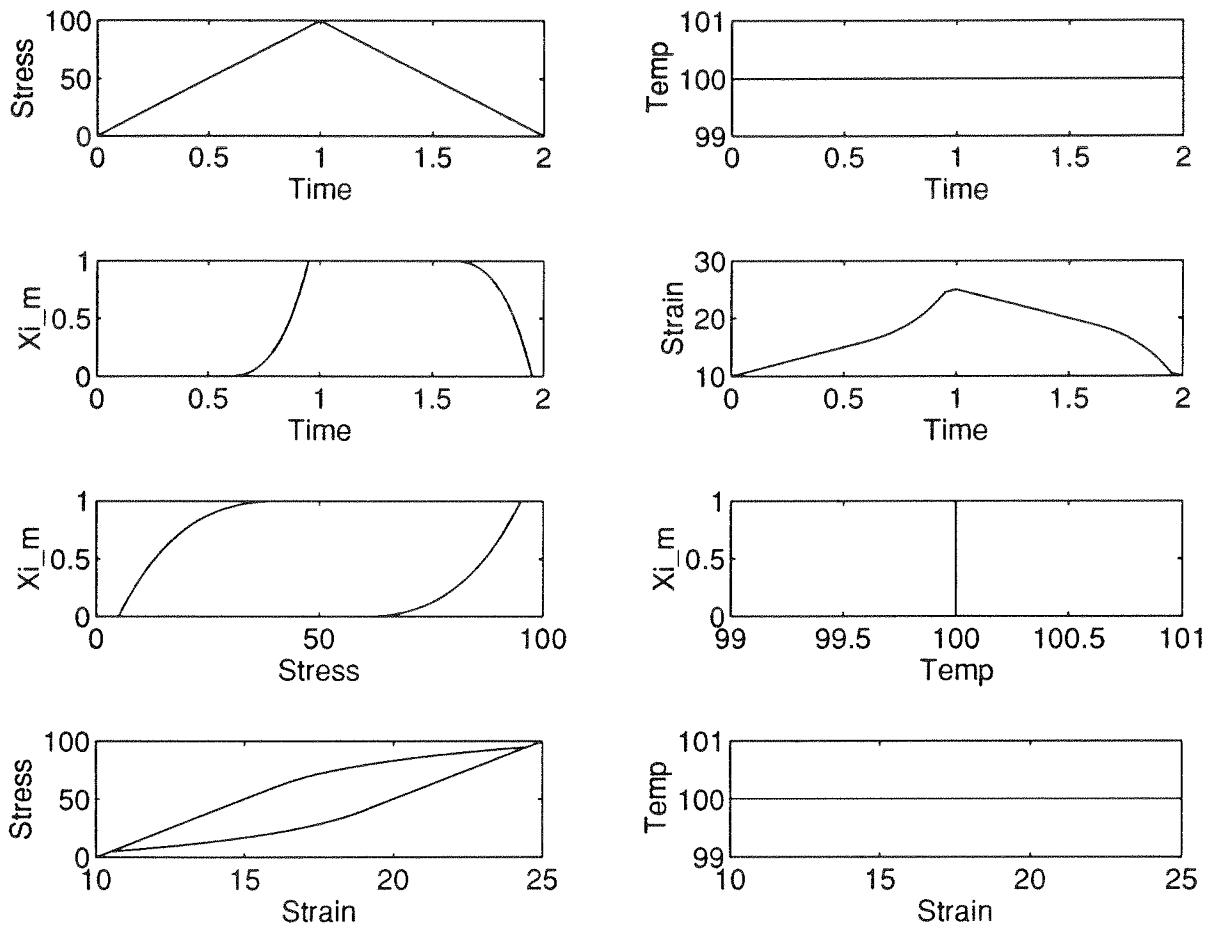

Figure 14: Speed parameter test. Larger values of the β-parameters correspond to slower transformations.