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A CONSTITUTIVE MODEL OF SHAPE MEMORY ALLOYS BASED ON VISCOPLASTIC LIKE EVOLUTION EQUATIONS

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Abstract

The paper presents a new model that allows the simulation of the macroscopic thermomechanical behavior of shape memory alloys (SMA). In this paper we present a description of the austenite-martensite phase transition, which takes into account the two types of martensite by introducing suitable internal variables: the volume fractions of the self-accommodating product phase (pure thermal effect) and the oriented (stress induced) product phase. The evolution equations of the internal variables are similar to the evolution equation in viscoplasticity. Differing from previous models, the presented one is able to model the behaviour of the SMA under combined thermal and mechanical loads. A numerical example is given that illustrates the ability of the model to capture the thermomechanical behavior of shape memory alloys under temperature change and proportional loadings.

Keywords: viscoplasticity, shape memory alloys, constitutive model, thermodynamical model.

1. Introduction

At present shape memory alloys (SMAs) are frequently used as one of the basic elements of intelligent structures and often cited as a typical example of smart materials with sensing, controlling, and actuating functions. The SMAs appear in a low (usually martensite) and a high temperature phase (austenite). In literature the shape memory effects (SMEs) are classified into the following three types: two way effect, one way effect and pseudo-elasticity. The effects can appear in this sequence with increasing temperature [8, 7, 6]. Due to intensive metallurgical investigations the microscopic mechanism of the shape memory effect has been disclosed. The thermomechanical behavior of SMAs is based on one or several of the following microscopic elementary processes: the austenite-martensite phase change, the reorientation of the martensitic plate, i.e. the transformation of one martensitic phase into another one that has a different crystallographic structure. Every grain of austenite in the polycrystalline body has its own orientation out of an infinite number of possible orientations. But each austenite grain component can be transformed into several martensite variants, whose orientations are determined

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[§] Tel. 0049-0721-6084186, email: *Levente.Juhasz@mach.uni-karlsruhe.de* by the orientation of the grain. In the case of Cu-based SMA the number of possible martensite variants of one austenite grain is 24.

At decreasing temperature the transformation from austenite into the self-accommodating martensite and under stress the transformation of austenite into the oriented martensite take place. From the crystallographic point of view, it is not possible to distinguish between self-accommodating and stress induced martensites. Nevertheless, their macroscopic effect on the shape of the SMA sample is different: The self-accommodating martensite does not produce any macroscopic phase transition strain, contrary to the oriented one. Both types of martensites can be present at the same time inside one SMA sample. Under mechanical loading, the transformation only forms such martensite variants which reduce the stress. If a mechanical load is applied on a martensitic grain, then the most suitable martensitic variants are generated from other variants of martensite. This effect is called reorientation.

The metallurgical basis of shape memory behavior is now well understood, and the research has been documented extensively in the literature for various alloy systems that undergo reversible martensitic transformations [14, 15, 11, 6, 7]. In the last decade, interest has risen in the constitutive modelling of these alloys, largely due to the growing applications of SMAs, in particular in the area of active material systems. The SMAs have to be described within the framework of non-equilibrium thermodynamics, because independent internal variables must be defined, to describe the internal processes in the non-equilibrium state.

We must choose a convenient number and type of internal variables. In this paper we use two scalar internal variables (see [9, 10]): The phase fraction (β^σ) of stress induced martensite, which is related to the creation of macroscopic phase transition strain, while the phase fraction (β^T) of the thermal induced martensite does not lead to macroscopic shape changes. Obviously, the internal variables chosen here are only averaged variables and do not describe the microscopic results of the phase transformation. The scalar internal variables limit the valid range of the model, because the scalar internal variable cannot describe the reorientation of the martensite. If we want to describe the behavior of SMAs under universal non-proportional mechanical loading, then we must use another set of internal variables (more in Section 3).

In several previous models an analogy to plasticity is accommodated [1, 9, 10, 5, 12]. The analogies are based on the existence of a condition of the transformation/plastic deformation. This condition can be written in the form of a yield surface, i.e. a critical stress with a temperature dependent hardening term.

In Section 3 we discuss the use of these two scalar variables for the phase fraction. We show the margin of a model with these variables concerning the reorientation of the martensite phases.

In the new model we propose an analogy to viscoplasticity, because we assume that the phase transformation takes place with a certain finite velocity, such that relaxation processes occur. The new evolution equations provide the possibility to calculate the time dependent effects.

We have modified the transformation surfaces of the Lexcellent model such that we can simulate the combined mechanical-thermal load (see numerical results in Section 6).

2. Formulation of the Constitutive Model

The model presented makes use of the classical local state postulate, which assumes the existence of a representative volume element (RVE) where internal variables can be defined. In the following, the elastic strain $\boldsymbol{\varepsilon}^e$, the temperature T, the volume fraction of self-accommodating martensite β^T and of oriented martensite β^σ are the state variables. Obviously, the following restrictions must be fulfilled:

$$\beta^\sigma \geq 0, \tag{1a}$$

$$\beta^T \geq 0, \tag{1b}$$

$$\beta^\sigma + \beta^T \leq 1. \tag{1c}$$

The total strain is assumed to be the sum of the elastic and transformation induced strains

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^{tr}. \tag{2}$$

In the case of linear elasticity the stress tensor is related to the elastic strains by

$$\boldsymbol{\sigma} = \boldsymbol{D}^e : \boldsymbol{\varepsilon}^e, \tag{3}$$

where $\boldsymbol{D}^e$ is the fourth-order elasticity tensor. In what follows, linear isotropic elasticity is assumed, such that

$$D^e_{ijkl} = \lambda\, \delta_{ij}\, \delta_{kl} + \mu\, (\delta_{ik}\, \delta_{jl} + \delta_{il}\, \delta_{jk}), \tag{4}$$

where λ and μ are the Lamé constants and δ is the Kronecker symbol.

Furthermore, we assume a proportionality between the phase transition strain and the volume fraction of the oriented martensite

$$\boldsymbol{\varepsilon}^{tr} = \boldsymbol{\kappa} \beta^\sigma. \tag{5}$$

In the case of isothermal pseudoelasticity (see LECLERG and LEXCELLENT [10]) the proportionality factor κ is

$$\boldsymbol{\kappa} = \frac{3}{2}\gamma \frac{\boldsymbol{s}}{\sigma_{eq}}, \tag{6}$$

where γ is the maximum of the pseudoelastic uniaxial strain (for complete phase transition) and does not depend on the temperature. The stress deviator $\boldsymbol{s}$ with $s_{ij} = \sigma_{ij} - \frac{1}{3}\, \sigma_{kk}$ and the von Mises equivalent stress σ_{eq} are also used in (6).

Here use will be made of the preceding relation, but writing it in rates, and assuming the case of proportional loadings. In this case the rate of the $\boldsymbol{\kappa}$ tensor is zero. One obtains

$$\dot{\boldsymbol{\varepsilon}}^{\boldsymbol{tr}} = \boldsymbol{\kappa} \dot{\beta}^\sigma. \tag{7}$$

3. Reorientation

The proportional loading in SMA can be guaranteed only with homogeneous stress fields. The inhomogeneous stress field, which would be proportional under elastic material behaviour, generates an SME which changes the stress situation. At this change the postulate of proportional stress is not valid. Hence we can use these models with the postulate of proportional loading only for simple geometries.

In this section we discuss the possibility of extending this model to the case of the non-proportional loading. With the assumption of the case of non-proportional loading and isothermal pseudoelasticity, we can write the rate form of the *Eq.* (5) as follows

$$\dot{\boldsymbol{\varepsilon}}^{tr} = \boldsymbol{\kappa}\dot{\beta}^{\sigma} + \dot{\boldsymbol{\kappa}}\beta^{\sigma}, \tag{8}$$

where the first term on the right hand side means the change of $\boldsymbol{\varepsilon}^{tr}$ with the martensitic transformation, the second term means the change through the stress direction. The change of stress direction also induced a reorientation by small stress. However, the experiments have established that the martensitic reorientation has a critical stress.

This problem can be solved using an auxiliary function H, which constrains the transformation above this critical stress. In this case *Eq.* (5) is not valid, only the following rate form of the constitutive equation:

$$\dot{\boldsymbol{\varepsilon}}^{tr} = \boldsymbol{\kappa}\dot{\beta}^{\sigma} + \dot{\boldsymbol{\kappa}}\beta^{\sigma} H(\sigma_{eq} - \sigma_0), \tag{9}$$

where σ_0 is the critical stress and the function H is defined in (24b). Here the function H is used only in the second term, because the evolution equation of β^{σ} contains also this condition. Here we have to take note of the implicit use of $\dot{\boldsymbol{\varepsilon}}^{tr}$ as internal variable with the evolution equation (9).

This rate type constitutive equation can describe the SME under a non-proportional mechanical load. The problem is that the orientation of the martensite is defined by $\boldsymbol{\varepsilon}^{tr}$. The change of orientation depends on the stress and the stress rate. Hence we cannot describe the *clear reorientation* in the case of constant load direction ($\dot{\boldsymbol{\kappa}} = \mathbf{0}$ and $\sigma_{eq} > \sigma_0$), which does not correspond to the orientation of the martensite. Let the status be totally martensitic ($\beta^{\sigma} = 1$, $\dot{\beta}^{\sigma} = 0$). If the state is totally martensitic then $\dot{\boldsymbol{\varepsilon}}^{tr} = \mathbf{0}$, but the reorientation is required.

An answer to this problem can be the systematic use of the $\boldsymbol{\varepsilon}^{tr}$ as internal variable instead of β^{σ}. In this case the definition of the evolution equation of the $\boldsymbol{\varepsilon}^{tr}$ is needed using transformation conditions and a thermodynamical force and they must not violate the thermodynamical laws. A model with these internal variables can describe the SME under general non-proportional loads, because it contains the direction of martensitic orientation independent of the stress.

The quantity of the oriented martensite β^{σ} can be defined as a function of the scalar invariants of $\boldsymbol{\varepsilon}^{tr}$ by

$$\beta^{\sigma} = f(\boldsymbol{\varepsilon}_{I}^{tr}, \boldsymbol{\varepsilon}_{II}^{tr}, \boldsymbol{\varepsilon}_{III}^{tr}), \tag{10}$$

and we can calculate the end of the transformation, see (1).

We can establish that the models with two scalar internal variables, for example this model, can best describe the three-dimensional proportional loading. Worth noting is the assumption that the mechanical load is proportional which also constrains the geometry of the sample.

4. Helmholtz Potential, Second Law of Thermodynamics

The Helmholtz free energy of the three-phase system is chosen in the form

$$\Phi(\boldsymbol{\varepsilon}^e, T, \beta^T, \beta^\sigma) = (1-\beta)\Phi_1 + \beta^T\Phi_2 + \beta^\sigma\Phi_3 + \Delta\Phi, \tag{11a}$$

where $\beta = \beta^T + \beta^\sigma$ is the total volume fraction of the product phase (martensite). The term Φ_i $(i = 1, 2, 3)$ from (11a) is the free energy of the phase i, where 1,2,3 corresponds to the austenite, to the self-accommodating martensite and to the oriented martensite, respectively. *Eq.* (11b) gives an expression for the energies of the phases.

$$\Phi_i := u_0^i - Ts_0^i + \frac{1}{2\rho}\,\boldsymbol{\varepsilon}_i^e : \boldsymbol{C} : \boldsymbol{\varepsilon}_i^e + c_v\left[(T-T_0) - T\log\left(\frac{T}{T_0}\right)\right] \tag{11b}$$

The term $\Delta\Phi$ has been called *configurational energy* by RANIECKI et al. [13] and presents the interactions that appear between the phases, typically the incompatibilities between deformations. One of the characteristics of this energy is that it must disappear when only one phase is present in the material. Moreover, in the case of three phases coexisting, this term must take into account interactions between one phase and the two remaining ones, separately. Thus one can assume the following expression for the configurational energy

$$\Delta\Phi := \beta^T(1-\beta^M)\Phi^{12} + \beta^\sigma(1-\beta^M)\Phi^{13} + \beta^\sigma\beta^T\Phi^{23}, \tag{11c}$$

where Φ^{ij} are the interaction energies between phase i and j $(i = 1, 2;\ \ j = 2, 3)$. Because the two types of martensite do not differ from the physical point of view, we can write the following system

$$\begin{aligned} \Phi^{12} = \Phi^{13} &= \Phi_{it}, \\ \Phi^{23} &= \Phi_{it}^m > 0, \end{aligned} \tag{12}$$

where we assume that Φ_{it} and Φ_{it}^m are constant. As a consequence, the combination of (11c) and (12) leads to

$$\Delta\Phi = \beta^T\beta_{eq}^\sigma\Phi_{it}^m + \beta^M(1-\beta^M)\Phi_{it}. \tag{13}$$

Let us write the Clausius–Duhem inequality as follows:

$$\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \rho s\dot{T} - \rho\frac{d\Phi}{dt} - \frac{\boldsymbol{q}}{\dot{T}}\mathrm{grad}T \geq 0. \tag{14}$$

Here s is the specific entropy of the system and $\boldsymbol{q}$ the heat flux received by the system. Taking account of (2), we can write (14) as

$$\left(\boldsymbol{\sigma} - \rho\frac{\partial\Phi}{\partial\boldsymbol{\varepsilon}^e}\right) : \dot{\boldsymbol{\varepsilon}}^e \quad + \quad \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^{tr} - \rho\frac{\partial\Phi}{\partial\beta^\sigma}\dot{\beta}^\sigma - \rho\left(s + \frac{\partial\Phi}{\partial T}\right)\dot{T} \\ - \quad \rho\frac{\partial\Phi}{\partial\beta^T}\dot{\beta}^T - \frac{\boldsymbol{q}}{\dot{T}}\mathrm{grad}T \geq 0. \tag{15}$$

The inequality (15) must hold for any $\dot{\boldsymbol{\varepsilon}}^{tr}$ and $\dot{T}$. Thus one obtains the following state equations

$$\boldsymbol{\sigma} = \rho\frac{\partial\Phi}{\partial\boldsymbol{\varepsilon}^e} = \boldsymbol{C} : \boldsymbol{\varepsilon}^e, \qquad s = -\frac{\partial\Phi}{\partial T}. \tag{16}$$

Assuming that the thermal dissipation term is non-negative, one obtains the Clausius-Duhem inequality as

$$\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}^{tr} - \rho\frac{\partial\Phi}{\partial\beta^\sigma}\dot{\beta}^\sigma - \rho\frac{\partial\Phi}{\partial\beta^T}\dot{\beta}^T \geq 0. \tag{17}$$

Introducing (5) and dividing by ρ, (17) can be written as

$$\pi_\sigma^f\dot{\beta}^\sigma + \pi_T^f\dot{\beta}^T \geq 0, \tag{18}$$

where the thermodynamical forces π_x^f are defined as follows

$$\pi_\sigma^f = \frac{\gamma\sigma_{eq}}{\rho} - (1-2\beta)\,\Phi_{it} - \beta^T\Phi_{it}^m + \pi_0^f(T), \tag{19}$$

$$\pi_T^f = -(1-2\beta)\,\Phi_{it} - \beta^\sigma\Phi_{it}^m + \pi_0^f(T). \tag{20}$$

The term $\pi_0^f(T)$ is the chemical potential of the phase transition.

$$\begin{aligned} \pi_0^f(T) &= \Delta u - T\Delta s, \\ \Delta u &= u_0^1 - u_0^2 = u_0^1 - u_0^3, \\ \Delta s &= s_0^1 - s_0^2 = s_0^1 - s_0^3. \end{aligned} \tag{21}$$

The thermodynamical forces π_σ^f and π_T^f make sense only in the case of austenite $\Leftrightarrow$ martensite phase transition and not in the case of a reorientation of the self-accommodating martensite into the oriented one. In this case, obviously $\dot{\beta}^\sigma = -\dot{\beta}^T > 0$. Thus, (18) has the form

$$\pi_{T\sigma}^f\dot{\beta}^\sigma \geq 0, \tag{22}$$

where

$$\pi_{T\sigma}^f = \pi_\sigma^f - \pi_T^f = \frac{\gamma\sigma_{eq}}{\rho} - (\beta^T - \beta^\sigma)\Phi_{it}^m. \tag{23}$$

Here $\pi_{T\sigma}^f$ denotes the thermodynamical force associated with the reorientation of a self-accommodating product phase. The phase transition $\beta^\sigma \Rightarrow \beta^T$ is not possible.

5. System Evolution and Kinetics

The phase changes have a critical stress and a temperature, during which this process can go on. There is another limit by conditions too, namely that the transformation can go on, until another phase of the transformation occurs. The rate of change depends on the state of environment, for example if abruptly cooled under the critical temperature the martensite can come into existence more easily.

In this section we discuss the conditions and equations of transformation kinetics. We use special simple conditions and propose the analogy of viscoplasticity, i.e. we do not require the consistence condition of a phase change surface by the evolution law of internal variables. The rate of change depends on the distance to the surfaces of the condition of the phase transition.

In this work we use the type of transformation surfaces by BRINSON [3, 2]. In this paper the surfaces are straight lines in the space of temperature and equivalent stress (see *Fig.* 1).

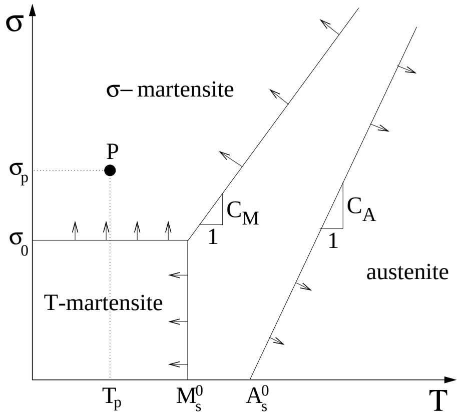

Fig. 1. Transformation surfaces

We can define these boundaries with the following five scalar material parameters.

- M_{s0}, A_{s0}, A_{s2} are the material parameters of the alloy, in usual notation.
- σ_0 is the critical equivalent stress at temperatures $T < M_{s0}$.
- c_M and c_A are the gradients of lines in the temperature-equivalent stress system.

Let us use the following notations:

$$\langle x \rangle = \begin{cases} x & \text{if} \quad x \geq 0 \\ 0 & \text{if} \quad x < 0 \end{cases}, \qquad ||\boldsymbol{x}|| = \sqrt{\frac{2}{3}\boldsymbol{x} : \boldsymbol{x}}, \tag{24a}$$

$$H(x) = \begin{cases} 1 & \text{if} \quad x > 0 \\ 0 & \text{if} \quad x \leq 0 \end{cases}, \qquad H^*(x) = \begin{cases} 1 & \text{if} \quad x \geq 0 \\ 0 & \text{if} \quad x < 0 \end{cases}. \tag{24b}$$

One of the advantages of these internal variables is that we can divide the phase change type into the following groups:

- phase changes of oriented martensite
  1. austenite ⇒ oriented martensite
  2. austenite ⇐ oriented martensite
  3. self-accommodating martensite ⇒ oriented martensite
- phase changes of self-accommodating martensite
  1. austenite ⇒ self-accommodating martensite
  2. austenite ⇐ self-accommodating martensite
  3. self-accommodating martensite ⇒ oriented martensite

We choose the evolution equations in the following form:

$$\begin{aligned}\dot{\beta^{\sigma}} &= K_1 \cdot H(1-\beta^{\sigma}) \cdot H(\pi^f_{\sigma}) \\ &\quad -K_2 \cdot H(\beta^{\sigma}) \cdot H(-\pi^f_{\sigma}), \\ &\quad +K_3 \cdot H(\beta^{T}) \cdot H(\pi^f_{T\sigma}) \qquad \text{(25a)} \\ \dot{\beta^{T}} &= L_1 \cdot H(1-\beta) \cdot H(\pi^f_{T}) \\ &\quad -L_2 \cdot H(\beta^{T}) \cdot H(-\pi^f_{T}) \\ &\quad -L_3 \cdot H(\beta^{T}) \cdot H(\pi^f_{T\sigma}), \qquad \text{(25b)}\end{aligned}$$

where K_i and L_i are the rate factors and the second factor in each line realizes the condition of the limit of phase quantities. The last factor in each line guarantees the positive dissipation. We define the rate factors of evolution equations by

$$\begin{aligned}K_1 &= k_1 \langle ||\boldsymbol{\sigma}|| - \sigma_0 \rangle \, H(M_{s0} - T) \\ &\quad + k_1 \langle ||\boldsymbol{\sigma}|| - \sigma_0 - c_M(T - M_{s0}) \rangle \, H(T - M_{s0}), \qquad \text{(26a)} \\ K_2 &= k_2 \left\langle T - A_{s0} - \frac{1}{c_A} ||\boldsymbol{\sigma}|| \right\rangle, \qquad \text{(26b)} \\ K_3 &= k_3 \langle ||\boldsymbol{\sigma}|| - \sigma_0 \rangle \, H(M_{s0} - T) \\ &\quad + k_3 \langle ||\boldsymbol{\sigma}|| - \sigma_0 - c_M(T - M_{s0}) \rangle \, H(T - M_{s0}), \qquad \text{(26c)}\end{aligned}$$

$$\begin{aligned}L_1 &= l_1 \langle M_{s0} - T \rangle \, H(\sigma_0 - ||\boldsymbol{\sigma}||), \qquad \text{(26d)} \\ L_2 &= l_2 \left\langle T - A_{s0} - \frac{1}{c_A} ||\boldsymbol{\sigma}|| \right\rangle, \qquad \text{(26e)} \\ L_3 &= l_3 \langle ||\boldsymbol{\sigma}|| - \sigma_0 \rangle \, H(M_{s0} - T) \\ &\quad + l_3 \langle ||\boldsymbol{\sigma}|| - \sigma_0 - c_M(T - M_{s0}) \rangle \, H(T - M_{s0}), \qquad \text{(26f)}\end{aligned}$$

where k_i, l_i are material parameters.

In this paper the phase change rate depends linearly on the distance of the current state to the phase transition surfaces. But the factors can also be defined as

$$K_i = \left(\frac{\Delta_i}{k_i}\right)^{n_i}, \tag{27}$$

where Δ_i means the distance and k_i and n_i are material parameters [4].

6. Numerical Results

We present the numerical results with the Lexcellent model [10] and compare them to the results of the new model. We carry out the numerical test first with the help of the computer algebra system MAPLE V.3.

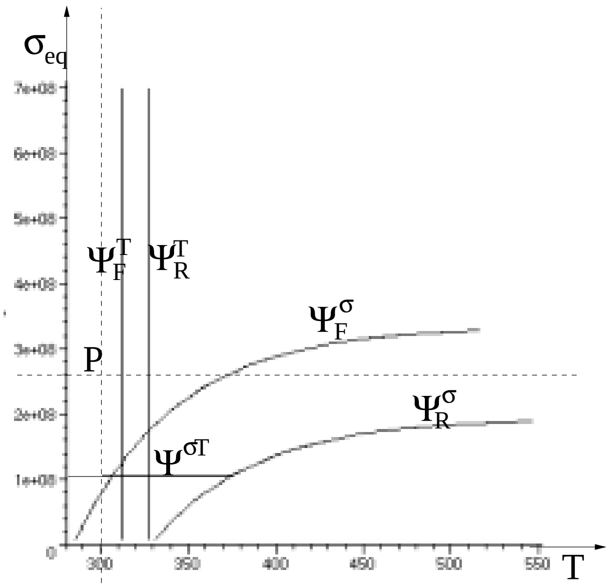

Fig. 2. Numerical computation of the transformation surfaces of the Lexcellent model

The transformation surfaces of the LEXCELLENT model (see *Fig.* 2) are similar to the new surfaces. In *Fig.* 2, $\Psi_{T/\sigma}^{F/R}$ means the transformation surface of the forward/reverse transformation of the self-accommodating martensite/oriented martensite, respectively. Here the surfaces do not appear in straight lines in the $\sigma - T$ space, because the definition of the surfaces are complex and have many material parameters. These transformation surfaces are incorrect under a combined thermal and mechanical load. A combined load (for example heating under stress) is unusual in the SME, but it appears in complex geometry with an inhomogeneous stress state. In this case the transformation is inhomogeneous in the cross section, which induces an internal stress. This stress induces a combined load via posterior heating. If the heating process starts in point P in *Fig.* 2, then at constant stress (a horizontal line) the state cannot cross the transformation surface Ψ_R^{σ} (surface of the reverse transition of the oriented martensite). But the experiments establish that the transformation appears at some temperature under a high stress, too.

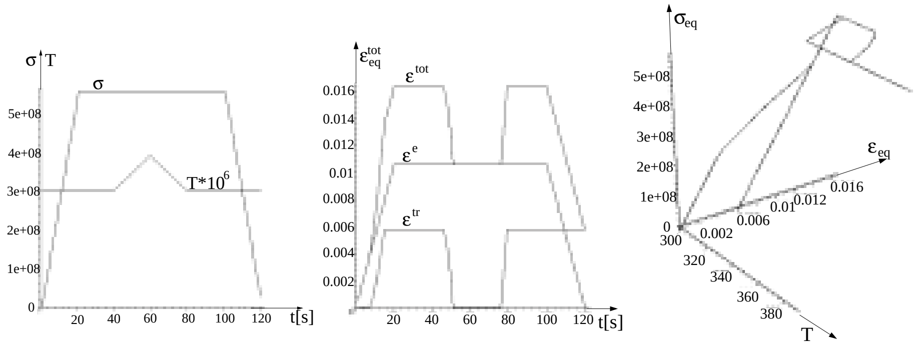

Fig. 3. Numerical results using the new model and complex loads

The numerical example shows (see *Fig.* 3) the behavior of the new model under complex loading. The first figure of 3 shows the load history. In the second picture, the total, the elastic and the transformation induced strain are plotted as a function of the time t. We observe the temperature induced martensite → austenite transformation under stress ($\varepsilon^{tr} \to 0$).

The increase of ε^{tr} for $t > 75$ shows that in this case the oriented martensite arises by cooling because of the mechanical load. The last figure shows the complete behavior of the SMA under this complex load in the $\varepsilon - \sigma - T$ space.

7. Conclusion

A new constitutive model of SMAs with numerical tests is presented. In this work the profitable features of the models of Lexcellent and Brinson [2, 10] are used. In the work only a few material parameters and simple transformation surfaces are defined. Hence the fitting of material parameters is easy. With these transformation surfaces we can simulate the behavior of SMAs under combined thermal and mechanical load, too. The model is valid in the case of proportional loading.

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