Constitutive modeling of shape memory alloys incorporating transformation-induced plasticity and damage

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Micro Abstract
Shape memory alloys (SMAs) are exploited in several innovative applications such as biocompatible actuators experiencing up to large number of cyclic loads. However, the description of the SMA cyclic response is still incomplete. The present work is devoted to propose a 3D model based on the thermodynamical coupling of different strain mechanisms such as the forward and reverse phase transformation, the martensitic reorientation, the transformation-introduced plasticity and fatigue damage.

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Introduction

Shape memory alloys (SMAs) are metallic materials with the unique capability of undergoing significant amount of deformation upon mechanical loading and retrieving their original shape through temperature increase. This characteristic is the result of the transformation at the scale of crystals between the two solid phases that the material adopts, the austenitic and the martensitic. The difference between these phases is due to the architecture of the crystalline structure, which varies between a cubic-like configuration in austenite and a less symmetric configuration in martensite [4,5]. Under cyclic loading the phase transformation mechanism is often accompanied by plastic and damage phenomena.

The present paper proposes a new 3D fully coupled thermomechanical phenomenological model for shape memory alloys, incorporating the irreversible mechanisms of transformation-induced plasticity (TRIP) and damage upon cyclic loading. A physical interpretation of the processes occuring inside a SMA grain is achieved by redefining the principles of the reorientation, the forward and the reverse transformation. This leads to the introduction of independent scalar variables that drive each of the three strain leading, reversible mechanisms of SMAs [1]. Both TRIP and damage mechanisms are considered to evolve during the forward or the reverse transformation. Accounting for these effects, a robust formalism is presented within a thermodynamical framework, and a proper Gibbs free energy potential is designed. The current model has been implemented in an open-source numerical simulation library [6] and the simulation of a complex thermomechanical loading path is conducted.

1 Description of deformation and damage mechanisms for SMAs

The various existing models that describe the phase transformation response of SMAs introduce, at least, two important internal variables: The martensitic volume fraction (MVF) ξ and the transformation stain ε^T [3]. The proposed model, taking into account the three different SMA mechanisms (forward - reverse transformation and reorientation), splits these two initial variables in the following manner:
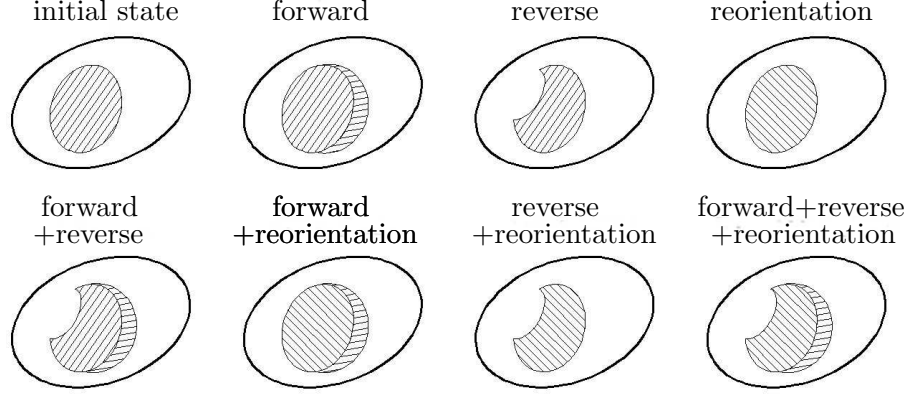
Figure 1. Schematic representation of possible states for a SMA macroscopic material point.

1. The rate of the total MVF $\dot{\xi}$ is assumed to be the result of two contributions, the rate of change of the MVF induced by forward and by reverse transformation, $\dot{\xi}^F$ and $\dot{\xi}^R$ respectively,

$$\dot{\xi} = \dot{\xi}^F - \dot{\xi}^R. \tag{1}$$

The minus in the right hand side of the last expression is due to the natural tendency of the MVF to be reduced during reverse transformation (transformation from martensite to austenite). Of course, ξ is restricted between the values of 0 and 1.

2. The rate of the total MVF transformation stain $\dot{\varepsilon}^T$ is decomposed in three terms, a forward $\dot{\varepsilon}^{TF}$, a reverse $\dot{\varepsilon}^{TR}$ and a reorientation strain rate $\dot{\varepsilon}^{RE}$,

$$\dot{\varepsilon}^T = \dot{\varepsilon}^{TF} + \dot{\varepsilon}^{TR} + \dot{\varepsilon}^{RE}. \tag{2}$$

3. The reorientation is considered as a mechanism similar to the kinematic hardening in plasticity. Thus, an additional variable $\boldsymbol{v}^{RE}$ is defined, which describes the hardening strain for reorientation.

The introduction of these volume fractions and strains permit significant freedom for the model to describe the various states that a SMA material point can obtain: pure forward transformation, reverse transformation and reorientation or different combinations (Figure 1).

The presence of TRIP and damage during the phase transformation mechanism (forward or reverse) introduce permanent irrecoverable deformation and stiffness reduction.

- The strain due to TRIP is accounted for by the following split of the rates of $\boldsymbol{\varepsilon}^{TF}$ and $\boldsymbol{\varepsilon}^{TR}$ is postulated,

$$\dot{\varepsilon}^{TF} = \dot{\varepsilon}^{TFT} + \dot{\varepsilon}^{TFP}, \qquad \dot{\varepsilon}^{TR} = \dot{\varepsilon}^{TRT} + \dot{\varepsilon}^{TRP}. \tag{3}$$

In the above expressions, $\boldsymbol{\varepsilon}^{TFT}$ is the reversible transformation strain and $\boldsymbol{\varepsilon}^{TFP}$ is the TRIP strain during forward transformation. The terms $\boldsymbol{\varepsilon}^{TRT}$ and $\boldsymbol{\varepsilon}^{TRP}$ represent similar strains for the reverse transformation. In addition to the strain tensors, scalar quantities similar to those of regular plasticity are introduced. Thus, $\dot{p}^F$ and $\dot{p}^R$ are the rates of the plastic strain accumulation during forward and reverse transformation respectively.

- The stiffness reduction is taken into account by the introduction of a damage variable d. To separate the damage accumulated during forwarn and reverse transformation, one can introduce two damage scalars, d^F and d^R with $\dot{d} = \dot{d}^F + \dot{d}^R$.

2 Thermodynamics based SMA model

The constitutive law of a material can be described using thermodynamic principles. A well designed thermodynamic potential requires the identification of proper observable and internal variables. For the SMA model proposed here, the designed Gibbs free energy potential is a function of the stress $\boldsymbol{\sigma}$, the temperature θ, the MVF ξ, the total transformation strain $\boldsymbol{\varepsilon}^T$, the damage variable d, the hardening strain for reorientation $\boldsymbol{v}^{RE}$, the transformation hardening function g^{TT} and the TRIP hardening function g^{TP}. Its form is

$$G = G_r + G_{ir}, \qquad \text{with} \quad G_r = (1 - \xi)G^A + \xi G^M + G^{mix} \quad \text{and} \quad G_{ir} = g^{TP}, \qquad (4)$$

where each term of the reversible part G_r respectively reads

$$G_r^i = U_0^i - s_0^i \theta + C^i \left[(\theta - \theta_0) - \theta \ln\left(\frac{\theta}{\theta_0}\right) \right] - \frac{1}{2(1-d)} \boldsymbol{\sigma} : \boldsymbol{S}^i : \boldsymbol{\sigma} - \boldsymbol{\sigma} : \boldsymbol{\alpha}^i (\theta - \theta_0), \quad (5)$$

$$G^{mix} = -\boldsymbol{\sigma} : \boldsymbol{\varepsilon}^T - \boldsymbol{\sigma} : +(1 + \lambda^{RE})\boldsymbol{X} : \boldsymbol{v}^{RE} + g^{TT}. \qquad (6)$$

In the above expressions, i stands for martensitic (M) or austenitic (A) phase. For each phase, C^i is the specific heat, $\boldsymbol{S}^i$ is the compliance tensor, $\boldsymbol{\alpha}^i$ is the thermal expansion coefficients tensor, U_0^i is the initial internal energy and s_0^i is the initial entropy. Moreover, $\boldsymbol{X}$ denotes the back stress of reorientation, λ^{RE} is a limiting cofactor for reorientation and θ_0 is a reference temperature.

In the framework of generalized standard materials the evolution laws of the nonlinear mechanisms are identified with the help of dissipation potentials or activation surfaces (like yield surface in plasticity). Each one of the three main mechanisms (forward, reverse transformation and reorientation) is connected with an activation surface [1]. The forward and reverse transformation surfaces include also the TRIP strains and the damage mechanism [2].

3 Numerical implementation

The numerical implementation of the SMA thermomechanical constitutive law is achieved in the form of a user material subroutine (UMAT) and is developed in the framework of an open-source numerical simulation library [6]. The UMAT subroutine is designed to be directly compatible with the FE commercial code ABAQUS and with the fully coupled thermomechanical analysis option.

The constitutive law nonlinear equations are solved with the use of the well known Return Mapping Algorithms and specifically the application of the Convex Cutting Plane technique. The activation surfaces, in the linearized form of the problem, are expressed through the Fischer-Burmeister method and they are checked simultaneously, avoiding with this way the numerically combersome Kuhn-Tucher inequlity conditions [1]. Moreover, except from the usual mechanical tangent stiffness tensor, three additional thermomechanical tangent moduli are evaluated that permit analyses under fully coupled thermomechanical conditions.

4 Numerical example

To illustrate the model capabilities, a numerical analysis is performed on a material point by considering complex thermomechanical, cyclic loading path. As illustrated in Figure 2, the normal stresses in the directions 1 and 2 and the temperature are varying in a cyclic, non-synchronized manner for a total time of 1800 s.

The numerical results (Figure 3) demonstrate the complicated thermomechanical response of the SMA material, which progressively through the cycles generate irrecoverable strain and presents a slight degradation of the elasticity modulus.
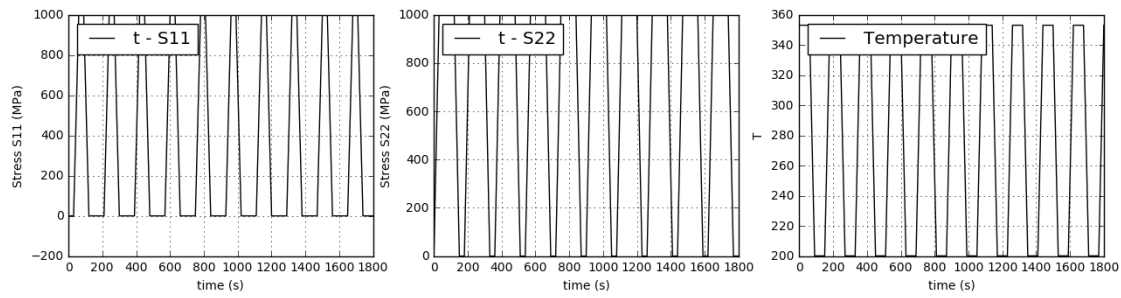
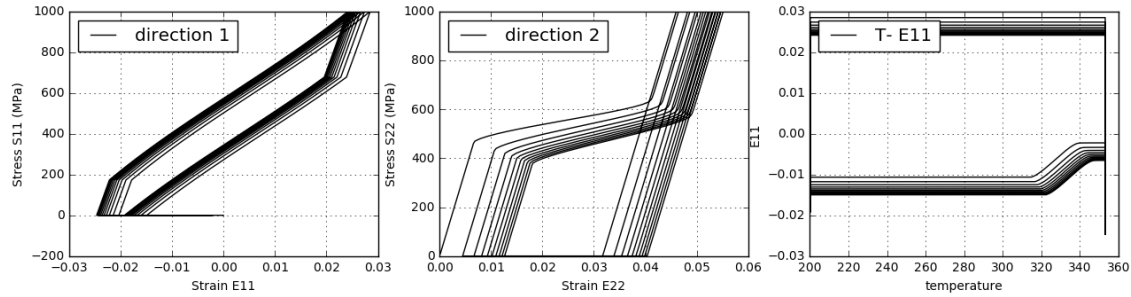**Figure 2.** Complex cyclic thermomechanical loading path for a SMA material.

Figure 3. Stress-strain and strain-temperature responses for the complex thermomechanical path.

Conclusions

The developed, fully coupled, thermomechanical model for SMAs is able to account for forward, reverse transformation and reorientation, TRIP and damage mechanism. An appropriate Gibbs free energy and a consistent thermodynamic framework allow to properly define the constitutive law and the evolution equations for the nonlinear mechanisms. The proposed model is very useful for understanding the SMA behavior under cyclic thermomechanical loading conditions and permits to analyze compicated responses. The development of the UMAT subroutine also gives the capability of the constitutive law to be integrated in structural applications through FE softwares.

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