An efficient method for solving the MAS stiff system of nonlinearly coupled equations: Application to the pseudoelastic response of shape memory alloys (SMA)

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Abstract. A Shape memory alloy (SMA) actuators have great potential in advanced technology applications where space, weight and cost are crucial design factors. They are known for the shape memory effect which is the ability to recover an initial configuration by simple heating after deformation. SMAs also exhibit a behavior called "pseudoelasticity" also known as "superelasticity" which is the shape recovery associated with mechanical loading and unloading at temperatures above specific values. The key characteristic of SMAs is the martensitic phase transformation, brought about by temperature change and / or by application of stress. Martensitic transformation is usually accompanied by significant changes in mechanical, electrical and thermal properties that render them as prime candidates for the development of smart structures and devices. This work is a contribution to the study of the influence of parameters such as operating temperature and the mode of heat transfer (natural or forced convection) on the pseudoelastic response of SMA used as actuators. Based on the mathematical formalism of the Müller, Achenbach and Seelecke model known as the "MAS model", we develop through a new mathematical formalism a new iterative resolution methodology of the coupled equations. The new approach provides very significant results and allows a significant gain in computation time.

1. Introduction
Shape memory alloys (SMAs) are a unique class of metal alloys that exhibit unusual properties such as shape memory effects (one-way and two-way shape memory effects), superelasticity (pseudoelasticity), damping effect, etc. Due to their specific characteristics such as the ability to cover large apparent permanent deformations (strains), lightweight and high work output, SMAs have been implemented in high-tech industries mainly as actuators or sensors. More recently, they have become candidates for microactuators when fabricated as thin films. These unique properties are related to a so called martensitic transformation (MT) which is brought about by temperature change and / or by application of stress. Martensitic transformation is between a high-symmetric cubic austenitic phase (A) and a low symmetric martensitic phase (M). MT is usually accompanied by significant changes in mechanical, electrical and thermal properties that render them as prime candidates for the development of smart structures and devices. External thermodynamic variables that affect the martensitic transformation are temperature and / or mechanical stress. MT can be activated by a thermal mechanical or thermomechanical cycle (loading / unloading) [1]. SMA actuators reliability and functionality depend on a good knowledge of these specific behaviors which must be properly
established mathematically and interpretable physically. SMAs exhibit a hysteretic nonlinear behavior with strong thermo-mechanical coupling. Temperature changes caused by latent phase transformation heats and Joule heating control explain the thermo-mechanical coupling. Thermo-mechanical behavior mathematical modeling and the martensitic transformation are very complex and still interesting scientific topics with innumerable scientific investigations [2]. Implementation in computer codes is difficult because of the representative elementary volume (REV) need [3]. In opposition, the so-called "phenomenological" models using macroscopic scale internal variables are best suited for computer codes implementation [4].

Generally, thermodynamic models are adapted for macroscopic responses capturing and allow explaining underlying physical phenomena. One of the most powerful and truly able to take into account both the strong thermo-mechanical coupling and the hysteretic nonlinearity models, is the model attributed to the authors (Müller - Achenbach and Seelecke) and known as "MAS model" [5,6]. Microscopic observations revealed that a SMA sample under a uniaxial load transforms into a twinned structure. Each twin is either in the austenitic phase denoted "A" or in a variant of the martensitic phase denoted "M+" or "M-". During the modeling, in addition to treating the nonlinearity problem, energy functions are introduced and associated to the different phases. Energies minima correspond to phases stability zones [7]. Temperature changes in the loaded SMA sample depend on latent heat emissions, phase changes absorptions, convection heat transfer on external surfaces and Joule heating. The mathematical formalism is based on statistical thermodynamics, probability of phase transition and latent heat. Thermodynamic laws application allows obtaining a coupled system of governing equations that describes the rate of change evolution of the present phases. Numerical solution of these coupled equations is very delicate and need very large machine time [8,9]. The present work is devoted to the development of a new efficient resolution methodology which will be used to study the influence of operating conditions on the pseudo-elastic response of a SMA sample used as activator. Conditions of use include the temperature and cooling mode.

2. The martensitic transformation mechanisms

The basic mechanism is a phase transition in the crystal lattice structure [10]. During a unidirectional loading, the SMA sample exhibits a twinned crystallographic structure (Figures 1 and 2). Both variants of the martensitic phase “M+” and “M-” can be mechanically interpreted as the results of the shear deformations of the crystal lattice of the parent austenite phase “A”. In the absence of external load, the martensitic phase is stable at low temperature while the austenite phase is stable at high temperature. Observation of a specimen during the phase transition reveals a structure of alternating layers of austenite and martensite. (Figure 2) illustrates the behavior of these layers in a tensile experiment. Initially, at low temperature, the body is in a martensitic state, half of the layers “M+”, the other half “M-”. At a critical load level, the “M-”-layers flip into the “M+”-phase, thus contributing to a considerable length change. Upon removal of the load, the “M-”-layers do not flip back into their original phase, but when the specimen is heated, all the layers transform into the austenitic phase. This causes the body to shorten again and thus gives rise to the well-known shape memory effect. Subsequent cooling finally completes the cycle by having the martensitic twins occur again.

3. MAS time-dependent thermomechanical behavior model

In order to describe the above behavior, the original MAS model takes the metallic layers as basic elements. For a representative elementary volume (REV), the microstructure of a sample consists of twins forming phases (martensite variants) “immersed” in a parent austenite phase.
Figure 1. Phases present in the martensitic transformation

Figure 2. The various stages of the martensitic transformation and the shape memory effect [9]

For a representative elementary volume (REV), internal variables denoted by $x_a$, $x_+$, and $x_-$ are associated and denote the volume fractions of the corresponding phases “A”, “M+” and “M-”.

Figure 3. The REV and the volume fractions of the phases

If we denote by $\Delta_a$, $\Delta$ and $\Delta_r$ the expectation values of the length changes in the phases calculated from statistical thermodynamics [18] (Heintze et al., 2008), we have:

$$
\begin{align*}
\Delta &= x_A \Delta_A + x_- \Delta_+ + x_+ \Delta_-\\
\end{align*}
$$

The rate of change of the phase fractions is given by the following equations:

$$
\begin{align*}
\dot{x}_+ &= -x_+ P^{+A} + x_A P^{A+} \\
\dot{x}_- &= -x_- P^{-A} + x_A P^{A-}
\end{align*}
$$

The quantities $P_{ab}$ are the transition probabilities from phase “a” to phase “b”, which also can be calculated from statistical thermodynamics. They’re functions of the parameters $x_A$, $x_+$, $x_-$ and $T$. For stress $\sigma$ and strain $\varepsilon$, it is clear that we have:

$$
\begin{align*}
\sigma &= \frac{\partial \Psi}{\partial \varepsilon} \\
\frac{\partial \sigma}{\partial \varepsilon} &= E
\end{align*}
$$

where $\Psi$ represents the considered effective potential energy and $E$ the elasticity modulus.

When incorporating the possibility of electric heating, which is crucial for an application as actuator, the energetic balance leads to:

$$
\rho c T = -\sigma_c S_v (T - T_0) + j(t) - (h_{M-} - h_A) x_+(t) - (h_{M+} - h_A) x_-(t)
$$

the above equation summarizes the different heat transfer phenomena affecting the SMA sample temperature $T$. 
To: the environment at temperature, \( \rho \) and \( c \) are respectively the density and the specific heat of the SMA sample, \( S \) the sample heat exchange surface. \( h_{M+}, h_{M-} \) and \( h_{A} \) are the specific enthalpies of the different phases. \( (h_{M+} - h_{A}) \) and \( (h_{M-} - h_{A}) \) represent the transformation latent heats of the two variants of martensite. \( j(t) \) the Joule heating \((-\alpha_{c}S_{v}(T - T_{0}))\) convection heat exchange and \( \alpha_{c} \) the thermal conductivity coefficient.

The equations (2) and (4) together with (1) constitute a stiff system of nonlinearly coupled ODEs:

\[
\frac{d}{dt} \begin{bmatrix} x_+ \\ x_- \end{bmatrix} \propto T = \begin{bmatrix} -p^{+A} & 0 & +p^{-A} & 0 \\ 0 & -p^{+A} & +p^{-A} & 0 \\ -(h_{M+} - h_{A}) & -(h_{M-} - h_{A}) & 0 & -\alpha_{c}S_{v} \\ 0 & 0 & 0 & j(t) + \alpha_{c}S_{v}T_{0} \end{bmatrix} \begin{bmatrix} x_+ \\ x_- \\ x_A \\ T \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \\ j(t) + \alpha_{c}S_{v}T_{0} \end{bmatrix}
\]

(5)

4. Stiff system algorithm resolution

By considering the notations:

\[
\frac{d}{dt} \begin{bmatrix} x_+ \\ x_- \rho \propto T \end{bmatrix} = \frac{d}{dt} \begin{bmatrix} Y \end{bmatrix} = \begin{bmatrix} -p^{+A} & 0 & +p^{-A} & 0 \\ 0 & -p^{+A} & +p^{-A} & 0 \\ -(h_{M+} - h_{A}) & -(h_{M-} - h_{A}) & 0 & -\alpha_{c}S_{v} \end{bmatrix} \begin{bmatrix} Y \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \\ j(t) + \alpha_{c}S_{v}T_{0} \end{bmatrix}
\]

(6)

\[
A(Y) = \begin{bmatrix} -p^{+A} & 0 & +p^{-A} & 0 \\ 0 & -p^{+A} & +p^{-A} & 0 \\ -(h_{M+} - h_{A}) & -(h_{M-} - h_{A}) & 0 & -\alpha_{c}S_{v} \end{bmatrix}
\]

(7)

And by introducing the initial conditions, we obtain:

\[
\begin{aligned}
\frac{d}{dt} \begin{bmatrix} Y \end{bmatrix} &= \lambda(Y) + \begin{bmatrix} Y \end{bmatrix} \\
\{Y(0)\} &= \{Y_{0}\}
\end{aligned}
\]

(8)

(9) is a nonlinear stiff initial value problem. Stiffness in this case comes from the difference in scale between different dynamic phenomena evolving simultaneously: volume fractions of the phases, latent heat and temperature \( T \). These conditions make it difficult to use conventional methods of resolution due to the very high number of integration steps and the associated convergence problems [11]. For the resolution we have developed a highly efficient algorithmic allowing us to apply the MAS model to the study of the pseudo-elastic response of SMA.

5. Results and Discussion

![Figure 4. Influence of the operating temperature on the hysteresis loop](image1)

![Figure 5. Influence of the heat exchange factor on the hysteresis loop](image2)
Figure 4 shows the clear influence of the operating temperature on the pseudo-elastic response of the SMA sample. Figure 5 shows that the SMA sample is not sensitive to the heat transfer mode. By analyzing the Figure 6, at low temperature (T = 10°C), the SMA sample consists mainly of the martensitic phase (80%), during the martensitic transformation this rate increases to the value of 95% and then stabilize around 100%.

6. Conclusion
The presented model was developed on the basis of the "MAS" model. It allows a very efficient way for analysing the pseudo-elastic response of a SMA sample for the manufacture of actuators. The mathematical formalism has allowed the development of a numerical simulation code. Obtained results are very significant and can reproduce the SMA pseudoelastic behaviour.

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