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Identification and interpretation of material parameters of a shape memory alloy (SMA) model

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Abstract. The thermomechanical behavior of Shape Memory Alloys (SMAs) is described by many micromechanical and phenomenological models. The first ones have material parameters whose physical meaning is based on the crystallography of the phase transformation related to the studied alloy. In contrast, phenomenological models often have material parameters whose physical meaning is not obvious and that makes them difficult to identify, some of which are based on mathematical considerations.

In this paper, we propose to use the formulation of the phenomenological model of Chemisky et al., and to consider the particular case of a superelastic SMA. In this case, the constitutive equation should be easily expressed analytically through the strain tensor as a function of applied load direction and material parameters. The behavior is then characterized by a complete and proportional loading. This analytical model contains 7 material parameters, 1 related to the elasticity and 6 to the phase transformation. Based on several isothermal tensile tests at various temperatures, material parameters of this model are identified using the Levenberg-Marquardt algorithm and an analytical calculation of the sensitivity matrix. Their physical meaning and their influence on the thermomechanical behavior of the studied alloy are highlighted and discussed.

Introduction

Identification of the material parameters of SMA constitutive models is a recurrent problem [1], which appeared with the first models. With each proposed model a rigorous identification procedure should systematically be associated. Otherwise, this should easily lead to either very bad results or artificially accurate results, neither of which being correct with respect to the adopted modeling framework. Constitutive models can be sorted into three categories according to the interpretation of their material parameters: the micromechanical models, the fully phenomenological models with mathematical approaches and the phenomenological models based on thermodynamic considerations. The last one can be placed between the two previous categories. Thermodynamic considerations allow matching each variable with a physical phenomenon [2]. The phenomenological approach makes the model adapted to FEM with a limited set of internal variables, and material parameters seem to be easier identified from macroscopic experimental data.

Identification of material parameters is usually conducted using uniaxial tensile tests at several temperatures in order to establish a phase diagram, with a graphic interpretation of experimental data [1]. It appears that inaccurate approximations are induced by this kind of identification. Moreover, several temperature-dependent parameters in a constitutive model are considered to be constant in the range of applications $\{-100 ; +150 \text{ }^\circ\text{C}\}$. That means that parameters identified at one temperature are slightly different from ones identified at other temperatures. It is difficult in this case to choose with rigor the optimized material parameters values.

In this paper, we propose to evaluate the error of identification by computing a cost function, which compares experimental data and the predicted values. Firstly, the prediction is performed with an analytical superelastic SMA model proposed by the authors containing 7 materials parameters. A Levenberg-Marquardt algorithm is then adopted to minimize this cost function [3,4]. This algorithm yields to an optimized set of material parameters. This optimized set is obtained with tensile tests at two temperatures. Numerical results are compared with experimental data at a third temperature.

SMA analytical model

In this study, the aim is to identify the parameters of an analytical SMA model. Such model gives the advantage to express explicitly the total strain in terms of the applied stress and material parameters. Thus, identification algorithm can be implemented analytically.

The main models describing the complex thermomechanical behavior of SMA require numerical resolution with implicit scheme. An explicit expression of the total strain imposes to describe a limited number of physical phenomena. It is chosen to identify the material parameters to describe superelastic behavior with an analytical model based on Chemisky et al. [2]. This one describes the behavior of a representative volume element (RVE), where four strain mechanisms contribute to the macroscopic strain response when a thermomechanical loading is applied: elastic strain $\boldsymbol{\varepsilon}^e$, thermal expansion $\boldsymbol{\varepsilon}^{th}$, martensitic transformation and orientation $\boldsymbol{\varepsilon}^T$, and accommodation of twins $\boldsymbol{\varepsilon}^{twin}$. The total strain $\boldsymbol{\varepsilon}$ is assumed to be additively decomposed into these four contributions. Both austenitic and martensitic phases are assumed to be isotropic and have the same thermoelastic constants. The transformation strain $\boldsymbol{\varepsilon}^T$ can be expressed as a function of the volume fraction of martensite f and the average transformation strain in the martensitic phase $\bar{\boldsymbol{\varepsilon}}_{ij}^T$ ($\boldsymbol{\varepsilon}_{ij}^T = f \cdot \bar{\boldsymbol{\varepsilon}}_{ij}^T$). In the superelastic domain the volume fraction of the self-accommodated martensite is equal to zero and thus the strain associated to the accommodation of twins $\boldsymbol{\varepsilon}^{twin}$ is null. The resulting analytical model tends to the Tanaka model [5].

$$f = \frac{\boldsymbol{\varepsilon}_{SAT}^T}{H_f} [\sigma - b_f(T - M_s)]. \quad (1)$$

In reverse transformation, the evolution of martensitic volume fraction is:

$$f = \frac{\boldsymbol{\varepsilon}_{SAT}^T}{H_f} [\sigma - b_r(T - A_f)]. \quad (2)$$

Considering the case of superelastic proportional loadings, Table 1 resumes the parameters that have to be identified.

Table 1. Physical interpretation of parameters to be identified for the superelastic behavior

E ,	Young modulus
b_f/b_r	Slope in the uniaxial stress-temperature diagram for forward/reverse transformation
$\boldsymbol{\varepsilon}_{SAT}^T$	Transformation strain magnitude in the direction of the transformation
M_s/A_f	Temperature for the {onset of forward/finish of reverse} transformation at zero stress
H_f	Transformation hardening parameter

Identification procedure

Experimental data have to be compared to numerical prediction obtained under the same conditions. In this study, isothermal tests have been conducted in the superelastic domain. They are stress-controlled and the stress field is assumed to be uniaxial. The evolution of the strain in the longitudinal direction according to the stress applied in the longitudinal direction is recorded.

The proposed model is able to predict the SMA behavior in the experimental test conditions. At each recorded stress value, experimental and predicted strain values can be compared. In this section, an identification procedure is developed. A cost function is proposed in order to quantify the difference between experimental and predicted values, based on a quadratic gap between them. In this work, two longitudinal strains are recorded. The cost function $C(p)$, with p the parameters, takes into account the data for each stress value, for two temperatures and for two longitudinal strains. This cost function can be applied in cases with several stress value, several temperatures, several strain components, and a general expression of this function is:

$$C(p) = \frac{1}{2} \frac{\sum_{T=T_1}^{T_Q} \sum_{t=t_1}^{t_K} \sum_{j=1}^n (\varepsilon_{xx}(p, T, t, x_j)^{num} - \varepsilon_{xx}(T, t, x_j)^{exp})^2}{\left(\sum_{T=T_1}^{T_Q} \sum_{t=t_1}^{t_K} \sum_{j=1}^n (\varepsilon_{xx}(T, t, x_j)^{exp})^2 \right)}, \quad (3)$$

where $\varepsilon_{xx}(T, t, x_j)^{exp}$ represents the longitudinal strain recorded at a material point j of coordinates x_j at the time t from an isothermal test performed at the temperature T . There are thus n material points considered for each time t . The value $\varepsilon_{xx}(p, T, t, x_j)^{num}$ represents the corresponding strain computed using a chosen constitutive model. p denotes the set of k guessed parameters.

The minimization of the cost function is conducted with the Levenberg-Marquardt algorithm [3,4]. The partial derivatives of the cost function with respect to the different material parameters are computed. The analytical formulae for the total strain provide analytical expressions of partial derivatives. This important point induces a robust and fast identification.

Results and discussion

To identify all the material parameters from experimental results, a minimum of two tensile tests are required to obtain the stress-temperature dependence (represented in the model to be identified by the parameters b_f and b_r) and to identify the model parameters. A third test is exploited for the experimental validation of the identification procedure.

The identification procedure has been validated on two various datasets. In each case, initial guessed values have been adopted, in a range where they have physical meaning. The first dataset is obtained on NiTi (50.6 at %Ni) dogbones specimens with three tensile tests at 323, 333 and 343 K. Specimens have been tested until failure, reverse transformation parameters cannot be identified. The second dataset is obtained on NiTi (50.8 at %Ni) wire specimens with loading-unloading tensile test at a strain rate of $3 \cdot 10^{-4}$ /s [6].

The Figure 1 shows the identification conducted on the first dataset. The predicted superelastic response is presented and compared to the three tension tests performed at 323 K, 333 K and 343 K, respectively. The red plots are the simulated response over the SMA at 323 K and 343 K, which corresponds to the experimental data utilized for the identification. The identified parameters values are listed in Table 2.

Table 2: Identified parameters with tensile tests at 323 and 343 K

E [GPa]	H_f [MPa]	ε_{SAT}^T	b_f [MPa/K]	M_s [K]
67.9	8.18	0.042	9.42	265

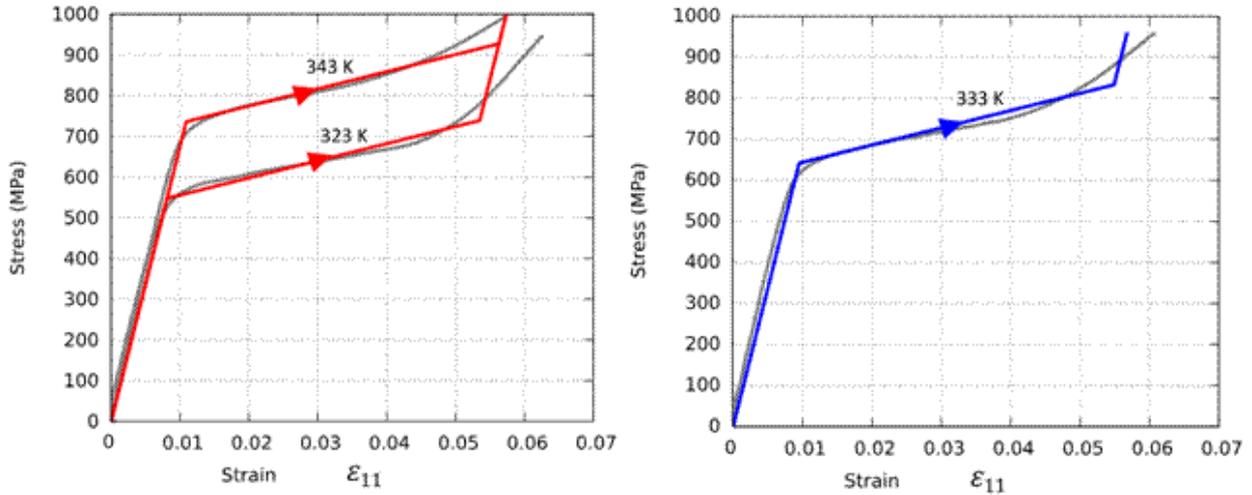


Figure 1. Comparison between the simulated response and the experimental data a) for isothermal tests at the two temperatures utilized in the parameter identification procedure (323 K and 343 K). b) Experimental validation for an isothermal test at 333 K.

The blue plot represents the prediction of the superelastic behavior at 333 K computed on the basis of the parameters previously identified at 323 K and 343 K. The predicted stress-strain curve is then compared with the experimental response. It can be seen that numerical prediction of stress evolution for the identification is very close to the experimental one. The comparison between experimental tensile test and numerical simulation at 333 K shows that identified parameters are reliable and can be utilized for the simulation of the superelastic response at various temperatures with a high accuracy.

The Figure 2 shows the identification conducted on the second dataset. Three isothermal superelastic tests were performed at $T = 313$ K, $T = 303$ K and $T = 298$ K. It can be seen that the beginning and the end of transformations (forward and reverse) are very smooth. This is due to the microstructure of the tested alloy and cannot be predicted with the adopted model. Indeed, the transformation hardening law is linear.

Initial parameters are taken to be the same as the set of parameters utilized in Chemisky et al. (2011). The identified parameters are given in Table 3. It can be seen that apparent Young modulus is lower than classical value for NiTi. It is explained by the smooth beginning and end of the transformation. The detection of critical stresses is affected, and the behavior described with Young modulus is not purely elastic. Figure 2a shows the simulation of the stress-strain curves based on this identification procedure at 298K and 313K. Figure 2b shows the simulation of an isothermal tension test at 303 K, which has not been used for the identification of the model parameters. It is shown that the identification procedure is able to obtain the model parameters that correspond to the behavior of the second dataset, and validate identification procedure.

Table 3: Identified set of parameters from uniaxial tests at 298K and 313K

E [GPa]	H_f [MPa]	ϵ_{sat}^T	b_f [MPa/K]	b_r [MPa/K]	M_s [K]	A_f [K]
24.5	3.3	0.032	5.42	4.0	257	273

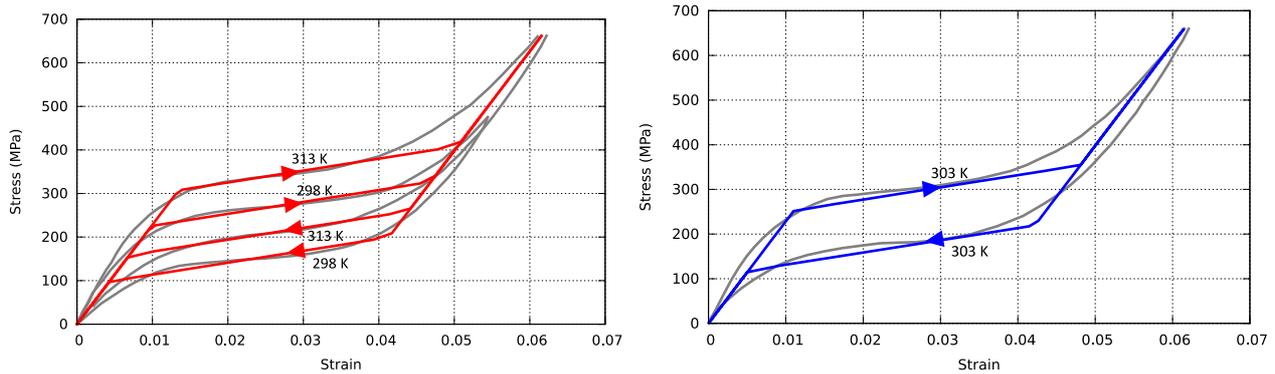


Figure 2. Comparison between simulation using the identified model parameters and the experimental response in uniaxial tension. Identification at 298 K and 313 K (a) and validation at 303 K (b).

Conclusion

In this study, an identification procedure adapted to a SMA model is proposed. This procedure is based on an inverse approach. An analytical model containing 7 material parameters predicts a SMA behavior and results are compared with experimental data. A cost function which takes into account the gap between experimental and predicted data is written, and minimized thanks to Levenberg-Marquardt algorithm. Material parameters are identified on two tensile tests at various temperatures, and the procedure is validated on a tensile test at a third temperature.

This identification procedure gives a powerful tool to rapidly exploit superelastic experimental tests data of a SMA, in order to conduct numerical simulations by modeling the thermomechanical behavior of this alloy. One limitation is the low number of parameter, which does not allow to model more complex phenomena as reorientation of martensite variants or traction-compression asymmetry. Further work will focus on identification procedure adapted to numerical SMA models.

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