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A MICROMECHANICAL MODEL FOR POLYCRYSTALLINE SHAPE MEMORY ALLOY WIRES INTEGRATED INTO SMART STRUCTURES

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ABSTRACT

This research aims at providing a computationally efficient one-dimensional micromechanical model for polycrystalline shape memory alloy (SMA) wires. The texture is described by a set of crystalline orientations along with their volume fraction. In the present work, each orientation relates to the martensitic transformation strain of its most favorably oriented martensitic variant (with respect to the loading direction), projected onto the wire axis. Two internal state variables characterize each crystalline orientation: the volume fraction of self-accommodated martensite, and the volume fraction of the most favorably oriented martensitic variant. The one-dimensional micromechanical model of the wire in traction thus considers the influence of the 3-dimensional texture. This model can describe superelasticity, self-accommodation and reorientation of martensite, as well as the one-way shape memory effect. It has been implemented numerically in a user-material subroutine (UMAT) for the finite element software ABAQUS, resorting to numerical constrained optimization tools. Several thermomechanical experiments on Nickel-Titanium wires have been carried out in order to identify the model parameters and the wire texture. The model can be used to simulate the response of morphing structures including SMA wires, actuated by shape memory effect.

KEYWORDS: SHAPE MEMORY ALLOY. POLYCRYSTALLINE WIRE.

INTRODUCTION

Thermomechanical models for shape memory alloys (SMA) can be categorized into phenomenological models and micromechanical models. Most micromechanical SMA models are 3-dimensional, computationally intensive and can only hardly be implemented in engineering codes to model smart structures. Some attempts at developing a simplified one-dimensional model have been made but often lack robustness [Nae, 2003]. The SMA behavior is usually modelled by using a free energy with constrained state variables, which makes the numerical implementation delicate. This research aims at providing a computationally efficient one-dimensional micromechanical model for polycrystalline SMA wires. The texture of Nickel-Titanium wires has been chosen in this study.

FORMULATION OF THE MODEL

The material is studied in form of a one-dimensional wire with n different possible grain orientations, the martensitic phase being under the form of lattice correspondent variants. We thus have the 12 different martensitic variants of the Nickel-Titanium alloy. Secondly, we make the assumption that each grain, when submitted to a load increment (mechanical or thermal) which is sufficient to trigger the phase change, deforms in the direction of its most favorably oriented martensitic variant [Shu, 1998]. This deformation will then be projected on the wire axis and represent the transformation strain. Each grain orientation i is characterized by its maximal phase transformation strain \( \varepsilon \), its self-accommodated martensite volume fraction \( \theta_{i} \), and its oriented martensite volume fraction \( \theta_{i} \) (the volume fraction of austenite in grain i is thus given by \( 1 - \theta_{i} - \theta_{i} \)). The following material parameters were adopted for the Nickel-Titanium wire:

- \( E \) the Young’s modulus (considered equal in all grains, in austenite as well as martensite variants)
- \( \lambda \) the latent heat term
- \( T_{0} \) a reference temperature
- \( G_{0} \) a dissipation parameter, corresponding to the self-accommodated martensite phase
- \( G_{i} \) a dissipation parameter, corresponding to the oriented martensite phase (with \( G_{0} < G_{i} \))

We model the thermomechanical behavior of the shape memory alloy by the following free energy:

\[
w(\varepsilon, \Theta, T) = \frac{1}{2} E (\varepsilon - \sum_{i=1}^{n} \theta_{i} \varepsilon_{i})^{2} + \lambda \frac{T - T_{0}}{T_{0}} \sum_{i=1}^{n} \left( \theta_{i} + \theta_{i} \right) \tag{1}\]

Where \( \varepsilon \) is the wire strain in the direction of traction and \( T \) is the wire temperature. The first term in (1) is the strain energy contribution, and the second term is the latent heat contribution. We adopt the framework of non-smooth thermodynamics [Fremond, 2001] and postulate the following dissipation potential which is convex and positive:

\[
\Phi(\dot{\Theta}) = \sum_{i=1}^{n} G_{0} |\dot{\theta}_{i}| + G_{i} |\dot{\theta}_{i}| \tag{2}\]

This model requires the determination of the parameters \( \varepsilon_{i} \) which we call texture parameters. They enable the model...
to capture the non-linear hardening effect at the end of the phase change on stress-strain curves (Figure 1).

**NUMERICAL IMPLEMENTATION**

For monotonic loading cases, it is possible to obtain analytical solutions, but complex loading paths require a numerical implementation of the problem. Writing down the time discretization of the equations leads to a nonlinear incremental problem. By means of a change of variables, it can be rewritten as a Linear Complementarity Problem (LCP) as it has been made in [Peigney, 2011] for a 3-dimensional monocrystal. In this case, we can take advantage of the sparsity of the resulting matrix and use interior-point algorithms to solve the LCP. We can thus obtain the updated internal variables $\theta_0$ and $\theta_1$ for a given load or temperature increment. The algorithm has been implemented on MATLAB, and a user-material subroutine based on this algorithm has been developed for the finite-element software ABAQUS, enabling to study structures containing SMA wires.

**EXPERIMENTAL VALIDATION**

The model has been compared to traction tests which have been carried out on SMA wires in a controlled temperature environment (a water bath). Before testing, the wire underwent thermomechanical cycling in order to test the stabilized behavior. More specifically, the non-linear hardening during the phase change (Figure 1) has been observed and exploited to obtain the texture parameters of the SMA. Constant stress experiments with thermal loading have also been realized, highlighting the shape memory effect.

![Simulation vs Experiment](image)

*Figure 1: Traction test on a SMA wire at 45°C and polycrystalline simulation with 50 grain orientations (MATLAB)*

**CONCLUSION**

A robust numerical SMA model has been formulated, numerically implemented and confronted to experimental data. It describes the main thermomechanical phenomena involved in shape memory alloys when used as actuators, but the model could be enhanced by developing a three dimensional version or by taking into account thermal expansion, the different elastic moduli of austenite and martensite, creep and stress relaxation, loading rate dependency, etc...

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