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Materials Science and Engineering A 481–482 (2008) 347–350

MATERIALS
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Experimental verification of a micromechanical model for polycrystalline shape memory alloys in dependence of martensite orientation distributions

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Received 17 May 2006; received in revised form 10 October 2006; accepted 26 October 2006

Abstract

We make use of a micromechanical model for polycrystalline shape memory alloys, whose main focus is the orientation distribution of the martensitic low symmetry variant. By energy minimization, the internal reorientation of martensite can be predicted. Hysteresis effects are included via the hypothesis that changes in the orientation distribution are connected to energy dissipation. From these considerations, we obtain evolution equations for the orientation distribution in terms of the thermomechanical driving forces. Comparing our model to results from synchrotron diffraction experiments, good agreement is found between experimentally observed and analytically predicted orientations of austenite and stress-induced martensite.

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Keywords: Micromechanical modeling; Polycrystals; Orientation distribution function; Reorientation of martensite; Driving forces; Shape memory alloys

1. Introduction

The focus of this paper is a comparison between analytical modeling and experimental testing of polycrystalline shape memory alloys. The material behavior is modeled based on the orientation distribution of the martensitic low-symmetry phase within the polycrystal. The model we use here has first been presented in [1]. By optimization of the global energy over all possible orientation distributions, we identify the thermodynamical driving forces as fundamental parameters governing the microstructural development. These driving forces are then compared to experimental results obtained by synchrotron diffraction experiments.

Details of the experimental procedure used are given in [2,3].

A first ansatz to model the material behavior of microstructured shape memory alloys by energy optimization has been presented in [4] and extended to include dissipative effects and inelasticity in [5]. A thermodynamical framework with a focus similar to this paper has been given in [6].

2. Micromechanical model

An ideal polycrystalline shape memory alloy consists of an infinite number of randomly oriented grains. For modeling purposes, however, the number of different crystal orientations is restricted to a large, but finite number *N*. Starting from an arbitrary fixed coordinate system, every crystal orientation *j* is described by a rotational tensor $\mathbf{R}_j$. Together with the linearized Bain strain $\boldsymbol{\varepsilon}_\mathrm{t}$ describing the transformation from the undeformed austenite reference configuration to the lower symmetry martensitic structure, the transformation strain for orientation *j* is

$$\boldsymbol{\eta}_j = \mathbf{R}_j^\mathrm{T} \boldsymbol{\varepsilon}_\mathrm{t} \mathbf{R}_j. \tag{1}$$

Here the arbitrary reference coordinate system has been chosen such that $\boldsymbol{\varepsilon}_\mathrm{t}$ is a diagonal matrix with entries $\varepsilon_{\mathrm{t}1}$, $\varepsilon_{\mathrm{t}2}$, and $\varepsilon_{\mathrm{t}3}$.

The volume fraction corresponding to the *j*th martensite orientation is now denoted by λ_j, $j = 1, \ldots, N$, whereas λ_0 corresponds to the transformation strain $\boldsymbol{\eta}_0 = \mathbf{0}$ of the austenite. Mass conservation then leads to the constraints

$$\lambda_j \geq 0, \quad \sum_{j=0}^{N} \lambda_j = 1, \quad j = 0, \ldots, N. \tag{2}$$

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doi:10.1016/j.msea.2006.10.218

We assume a simple linear elastic material law:

$$\Psi_j(\boldsymbol{\varepsilon}_j, \boldsymbol{\eta}_j) = \tfrac{1}{2}(\boldsymbol{\varepsilon}_j - \boldsymbol{\eta}_j) : \mathbb{A} : (\boldsymbol{\varepsilon}_j - \boldsymbol{\eta}_j) + \alpha_j, \tag{3}$$

where $\mathbb{A}$ is the elasticity tensor with components $\mathbb{A}_{klmn} = \Lambda\delta_{kl}\delta_{mn} + 2\mu\delta_{km}\delta_{ln}$, ":" means contraction with respect to two indices, and α_j denotes the chemical energy of the jth variant, which only differs from austenite to martensite but is the same for all martensite variants for reasons of symmetry. The isotropy of the elastic constants may be assumed for a polycrystalline material since anisotropies are averaged out for a sufficiently large number of randomly oriented grains. Isotropy is, however, not a necessary condition required in our model.

In the energy formulation (3), we introduced the strain $\boldsymbol{\varepsilon}_j$ of the crystals of orientation j. The global strain $\boldsymbol{\varepsilon}$ is then given as the average

$$\boldsymbol{\varepsilon} = \sum_{j=0}^{N} \lambda_j \boldsymbol{\varepsilon}_j, \tag{4}$$

which leads to the following formulation of the global energy for fixed volume fractions:

$$\Psi^{\text{rel}}(\boldsymbol{\varepsilon}, \boldsymbol{\lambda}) = \inf\left\{ \sum_{j=0}^{N} \lambda_j \Psi_j(\boldsymbol{\varepsilon}_j, \boldsymbol{\eta}_j) \,\middle|\, \boldsymbol{\varepsilon}_j, \boldsymbol{\varepsilon} = \sum_{j=0}^{N} \lambda_j \boldsymbol{\varepsilon}_j \right\}. \tag{5}$$

This way of calculating the free energy corresponds to a relaxation by convexification, which is actually a very crude way of obtaining lower bounds as estimates to the energy of a multivariant material. For more sophisticated ways of relaxing energy functions and the corresponding mechanical interpretations, see [7,8]. For a comparison of upper and lower bounds to the free energy in order to estimate the quality of the convexification bound, see [9–11].

Minimizing (5) over the crystal strains $\boldsymbol{\varepsilon}_j$ yields the straightforward expression for the relaxed energy

$$\Psi^{\text{rel}}(\boldsymbol{\varepsilon}, \boldsymbol{\lambda}) = \frac{1}{2}(\boldsymbol{\varepsilon} - \boldsymbol{\eta}_{\text{eff}}) : \mathbb{A} : (\boldsymbol{\varepsilon} - \boldsymbol{\eta}_{\text{eff}}) + \alpha_{\text{eff}}, \tag{6}$$

with the effective transformation strain and chemical energy

$$\boldsymbol{\eta}_{\text{eff}} = \sum_{j=0}^{N} \lambda_j \boldsymbol{\eta}_j \quad \text{and} \quad \alpha_{\text{eff}} = \sum_{j=0}^{N} \lambda_j \alpha_j. \tag{7}$$

The crystal strains for which this minimal energy is achieved are

$$\boldsymbol{\varepsilon}_j = \boldsymbol{\varepsilon} + \boldsymbol{\eta}_j - \boldsymbol{\eta}_{\text{eff}}. \tag{8}$$

3. Time evolution

In order to fully describe the material behavior, an ansatz for the dissipation within the polycrystal is needed. Since changes in the orientation distribution correspond to a growth and shrinking of domains containing certain variants, an intuitional assumption is the dissipation function

$$\Delta(\dot{\boldsymbol{\lambda}}) = r|\dot{\boldsymbol{\lambda}}| \tag{9}$$

which connects the Euclidian norm of the rate of change of the orientation distributions linearly to the dissipated energy. A discussion of different dissipation functions in micromechanical and multiscale models for shape memory alloys may be found in [12].

To derive the evolution equations, we start from the minimum principle

$$\mathcal{L}_{\boldsymbol{\varepsilon},\boldsymbol{\lambda}}(\dot{\boldsymbol{\lambda}}) = \frac{\mathrm{d}}{\mathrm{d}t}\Psi^{\text{rel}}(\boldsymbol{\varepsilon}, \boldsymbol{\lambda}) + \Delta(\dot{\boldsymbol{\lambda}}) \rightarrow \min \quad \text{under the constrains (2).} \tag{10}$$

A mathematically identical formulation has been derived in [13], however in a mechanically different setting.

Furthermore, we introduce the thermodynamically conjugate driving forces to $\dot{\boldsymbol{\lambda}}$

$$q_j = -\frac{\partial \Psi^{\text{rel}}}{\partial \lambda_j} = \boldsymbol{\eta}_j : \mathbb{A} : (\boldsymbol{\varepsilon} - \boldsymbol{\eta}_{\text{eff}}) - \alpha_j. \tag{11}$$

Variational calculus and a Legendre transform with respect to the driving forces then yield the evolution equation

$$\dot{\boldsymbol{\lambda}}_{\mathcal{A}} = \rho\, \text{dev}_{\mathcal{A}} \mathbf{q}_{\mathcal{A}} \tag{12}$$

constrained by (2) and the Kuhn–Tucker conditions

$$\rho \geq 0, \quad \Phi(\mathbf{q}) = |\text{dev}_{\mathcal{A}} \mathbf{q}_{\mathcal{A}}| - r \leq 0, \quad \rho\Phi = 0. \tag{13}$$

Here we have introduced the notions of an *active set* $\mathcal{A} = \{j | \lambda_j > 0\}$ and its *active deviator* $\text{dev}_{\mathcal{A}} \mathbf{x}_{\mathcal{A}} = \mathbf{x}_{\mathcal{A}} - (\sum_{\mathcal{A}} x_j) \mathbf{1}_{\mathcal{A}}/n$, n being the number of elements of the active set and $\mathbf{1}_{\mathcal{A}}$ the n-vector with 1 in every entry. The index $\mathcal{A}$ means the restriction of an $(N+1)$-vector to the active set $\mathcal{A}$.

A more detailed derivation of this model is given in [1,14].

4. Examples

The ability of the procedure presented above to model the most important effects in the behavior of polycrystalline shape memory alloys, such as pseudoelasticity and the shape-memory effect, has been shown in [1,14]. In this work, we focus on the comparison of analytically and experimentally obtained orientation distributions.

In Eq. (11), the term

$$\boldsymbol{\sigma} = \mathbb{A} : (\boldsymbol{\varepsilon} - \boldsymbol{\eta}_{\text{eff}}) \tag{14}$$

equals the global stress. From experimental observations and analytical results obtained with the model presented above, it is known that the transformation between austenite and martensite mainly takes place in the plateau where the stress is approximately constant. Consequently, the driving forces and thus, following Eq. (12), also the growth rates of the domains of certain orientations are constant over the whole plateau in which the transformation takes place. For a qualitative comparison, we may therefore assume that the probability of finding a certain orientation of the martensite is proportional to the corresponding driving force, hence

$$\lambda_j = \max\{0, k_1(\boldsymbol{\eta}_j : \boldsymbol{\sigma} - k_2)\} \quad \text{for } j \neq 0, \tag{15}$$

for appropriate constants $k_1, k_2 > 0$.

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