

## MICROMECHANICAL MODELLING OF PSEUDOELASTIC SMA POLYCRYSTALS UNDER NON-PROPORTIONAL LOADING

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### 1. Introduction

This work is concerned with micromechanical modelling of polycrystalline shape memory alloys (SMA) undergoing stress-induced martensitic transformations. In our previous papers [1, 2, 3], a micromechanical model of stress-induced phase transformation in SMA single crystals has been developed, starting from transformations of the atomic lattice structure and using exact compatibility conditions on the interfaces. In this model, sequential application of the micro-macro transition for rank-one laminates combined with a local phase transformation criterion provides overall response of a single crystal of a higher-rank laminated microstructure varying with the overall deformation. The transformation criterion is rate-independent with a threshold value for the thermodynamic driving force acting on a phase transformation front, including in this way the intrinsic dissipation due to phase transition. Selection of an optimal microstructure for the actual type of loading, from a number of different possibilities, is based on the transformation criterion, and the corresponding procedure can be interpreted as minimization of the incremental energy supply [4]. That approach is extended here to the scale of a polycrystalline aggregate, with the focus on the effect of interaction between neighbouring grains. The proposed grain-to-polycrystal transition scheme bears a resemblance to that developed recently in [5] in a different context, namely, for the prediction of texture development in plastically deforming metals.

### 2. Multi-scale model

The stress-induced martensitic transformation is assumed to proceed by the formation and evolution of microstructure at several scales, starting from the scale of the crystalline lattice, through the intermediate scales of martensite–martensite and austenite–martensite laminates, up to the scale of a single grain with complex multi-variant martensitic microstructures. The response of a single grain is fully defined by specifying the average Helmholtz free energy  $\bar{\phi}$  (e.g. [6]) and dissipation function  $\bar{D}$ . Selection of the active transformation mechanisms, i.e. the evolution of the microstructure, is then performed by minimization of the incremental energy supply [4],

$$(1) \quad \Delta E \rightarrow \min \quad \text{subject to kinematical constraints,}$$

where  $\Delta E = \Delta \bar{\phi} + \Delta \bar{D} + \Delta \Omega$ , the prefix  $\Delta$  denotes a virtual increment from a given state, corresponding to a given increment of an external control parameter, and  $\Delta \Omega$  is the increment in the potential energy of external loads.

In order to realistically describe the pseudoelastic response on non-proportional loading paths, the dissipation is assumed to comprise two components,

$$(2) \quad \Delta \bar{D} = f_c |\Delta \bar{\eta}| + f_r |\Delta \bar{\eta}_r|,$$

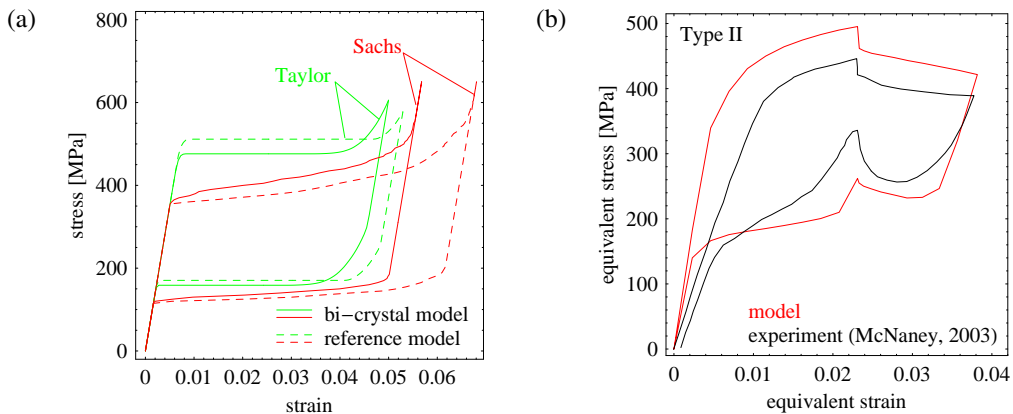
associated with the increment  $\Delta \bar{\eta}$  in the volume fraction of martensite due to the forward or reverse austenite–martensite transformation, and with the volume fraction  $\Delta \bar{\eta}_r$  of reoriented martensite.

Interaction of grains is accounted for by assuming that the polycrystal is an aggregate of bi-crystals, each formed by a grain boundary, of fixed orientation, and by parts of two adjacent grains.

Compatibility conditions (equilibrium and displacement continuity) on the grain boundary are enforced on the average stresses and strains within each sub-grain. The average stress and strain of a bi-crystal can be further averaged over the aggregate of differently oriented bi-crystals using any of the available grain-to-polycrystal transition schemes. At this stage, the effect of crystallographic texture can be easily included in the model by choosing preferential orientations of the grains.

### 3. Model predictions

The model has been applied to predict the pseudoelastic response of polycrystalline NiTi on proportional and non-proportional loading paths. Sample results are presented in Fig. 1. For instance, from Fig. 1(a) it is seen that the bounds corresponding to the Taylor and Sachs models are significantly improved when these schemes are combined with the bi-crystal model.



**Figure 1.** Predictions of the pseudoelastic response of polycrystalline NiTi for (a) uniaxial compression and (b) non-proportional tension–torsion loading (compared to the experimental results of McNaney et al. [7]).

**Acknowledgement** This work was supported by the KMM-NoE project.

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