

# THEORY AND COMPUTATION OF QUASIPLASTIC AND SUPERELASTIC MARTENSITIC PHASE TRANSFORMATIONS – COMPLAS VIII

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**Key words:** Martensitic Phase Transformation, Convexification, Validation.

**Summary.** *A survey and refined numerical treatment with validation of test results is presented for a rate-independent macroscopic unified PT material model including mass conservation with respect to phase fractions and convexified free energy. Special attention is given to temperature dependent PTs.*

## 1 INTRODUCTION

Phase transformation (PT) from austenite to martensite is activated by cooling the material below the martensite start temperature  $M_s$  or by mechanical loads above an adequate critical stress invariant. By cooling below  $M_s$  martensite twins are formed which become detwinned due to subsequent mechanical loading.

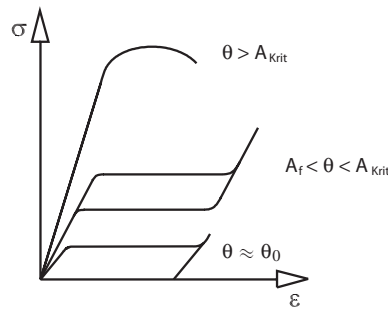


Figure 1: Stress-strain responses of a shape memory alloy at different temperatures.

In case of so-called quasiplastic deformation, caused by external loadings leading to detwinning, it can only be reversed by heat supply.

However, at the event of loading at high temperatures above the austenite finish temperature  $A_f$ , the transformation of austenite into oriented martensite takes place without intermediate martensite twins. For subsequent unloading below a second critical stress invariant, the reverse transformation from martensite into austenite takes place. This

behavior is called superelastic (or pseudoelastic) because the strain goes back to zero after unloading, but the stress-strain curve shows a stress-plateau in the region where PT occurs. It should be pointed out that this property only holds within a restricted temperature range. At too large temperatures ( $\theta > A_{Krit}$ ) it turns out that plastic deformation of austenite needs lower strain energy than forming martensite, fig. 1.

## 2 A UNIFIED MACROSCOPIC MATHEMATICAL MODEL FOR PHASE TRANSFORMATIONS OF MONOCRYSTALS

The total strain energy density of a crystal consists of the partial energies of each phase. According to the 1. and 2. laws of thermodynamics the actual phase is formed according to the minimum total energy density. Therefore austenite is the stable phase at  $\theta > A_s$  because it has the lowest energy under this condition, whereas martensite is the privileged phase at  $\theta < M_s$ .

The classical phenomenological thermomechanical theory of a macro-continuum with  $C^1$ - continuous point kinematics is applied. It is based on Bain's principle postulating that the martensitic crystallographic structure is achieved along the smallest lattice strain. Moreover, martensite is formed with respect to an habit plane without rigid rotation and strains.

The phases are called compatible in case of small stresses in the habitus plane at the interface of two phases. If the stresses at the interface are too large the phases are incompatible. The number of possible martensite variants is restricted by the condition that two neighbored phases can only exist if they are compatible.

The austenite and martensite crystallographic lattices and their deformations are described by Bravais lattices, using adequate linear independent lattice vectors. According to the Cauchy-Born hypothesis, the deformation of the Bravais lattice vectors can be presented by the deformation gradient  $\mathbf{F}$ ,  $\mathbf{F} \neq \mathbf{0}$  of the point continuum.

A unified mathematical model with a related numerical method is used in this paper as presented by Govindjee and Miehe in 2001 [2], based on the assumption by Ball and James [1] that the macroscopic strain energy  $\Psi(\boldsymbol{\varepsilon})$  of a crystal corresponds to the minimum of the energies of all possible phase variants, given by

$$\Psi(\boldsymbol{\varepsilon}) = \min_{i=1..n} \left[ \frac{1}{2}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_i^t) : \mathbb{C}_i : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_i^t) + A_i \right] , \quad (1)$$

with the linearized strain tensors  $\boldsymbol{\varepsilon}$  and  $\boldsymbol{\varepsilon}_i^t$ . The term 'unified model' means the extension of the Helmholtz free energy to a Lagrangean functional, as already introduced in [3] by Patoor et al. for a two-phase material. The added constraint concerns the explicit mass conservation of the phases.

The quasi-convexified free energy is presented as

$$\Psi(\boldsymbol{\varepsilon}, \boldsymbol{\xi}) = \boldsymbol{\xi} \cdot \boldsymbol{\psi}(\boldsymbol{\varepsilon}) + \Psi^M(\boldsymbol{\xi}) , \quad (2)$$

with the vector of phase fractions  $\boldsymbol{\xi} = \sum_{i=1}^n \xi_i \mathbf{e}_i$ ;  $\boldsymbol{\psi}$  is the column vector of phase energies as

$$\boldsymbol{\psi} = \sum_{i=1}^n \psi_i \mathbf{e}_i \quad , \quad \mathbf{e}_i \in \mathbb{R}^n \quad . \quad (3)$$

Evolution equations can be derived from a Lagrangean functional with the above described constraints in the form

$$\mathcal{L}(\boldsymbol{\varepsilon}, \boldsymbol{\xi}, \boldsymbol{\gamma}, \delta) = \Psi(\boldsymbol{\varepsilon}, \boldsymbol{\xi}) - \boldsymbol{\gamma} \cdot \boldsymbol{\xi} + \delta(\mathbf{e}^* \cdot \boldsymbol{\xi} - 1), \quad (4)$$

with the vector  $\boldsymbol{\gamma}$  and the scalar  $\delta$  of Lagrangean parameters for the  $n$  phases fulfilling the Kuhn-Tucker conditions

$$\boldsymbol{\gamma} \geq 0 \quad \text{und} \quad \boldsymbol{\gamma} \cdot \boldsymbol{\xi} = 0. \quad (5)$$

The energy dissipation condition for the driving force  $\mathbf{f} = \partial \mathcal{L} / \partial \boldsymbol{\xi}$  and a local maximum dissipation principle read

$$\mathcal{D} = \mathbf{f} \cdot \dot{\boldsymbol{\xi}} \geq 0 \quad , \quad \mathbf{f} \cdot \dot{\boldsymbol{\xi}} \rightarrow \max \quad . \quad (6)$$

With analogies to the theory of elastoplasticity it follows that the 'transformation function'  $\phi$  is convex (similar to a convex yield function) according to

$$\phi = \|\mathbf{f}\| - f_c \leq 0 \quad . \quad (7)$$

Iterative time integration of the constitutive equations is performed by Newton's method in each integration point of the spatial finite elements; the corresponding C-routine is connected with Abaqus via the UMAT-interface.

### 3 NUMERICAL MODEL-VALIDATION OF STRAIN CONTROLLED 1D TENSION EXPERIMENTS

Uniaxial tension experiments were carried out by Xiangyang et al. [4] with rod specimens having rectangular cross-sections, made from  $\text{Cu}_{82}\text{Al}_{14}\text{Ni}_4$  monocrystals . Two types of specimens were investigated therein, the first showing the shape memory effect (SME) with quasiplastic deformations, and the second one deforming with superelasticity (SE). *Specimen with SME:* Phase fraction histories of all phases were computed at an integration point in the middle of the specimen. Austenite degenerates and the martensite variant 6 arises. After complete unloading both phases exist unchanged due to their thermodynamic equilibrium state. If the specimen would be heated up to a temperature  $\theta > A_f$  the material would return to its initial (austenitic) state because it is the only stable state

under those conditions.

*Specimen with SE:* In contrast to the SME-specimen the SE-specimen shows a reverse transformation from martensite to austenite, because martensite is not stable at 293 K and thus transforms back for unloading, combined with vanishing large PT-strains which motivates the term 'superelastic' deformation behavior.

The **comparison between experimental and numerical results** are presented in fig. 2 a) and b). Both figures show that the applied macro-model for phase transformation describes the experimental results very well, regarding the upper bounds of the stress. It is also obvious from fig. 2 a) that an appropriate micro-model of PT for describing the experimental stress-strain curve needs crucial micro-physical information and process data which are hardly available.

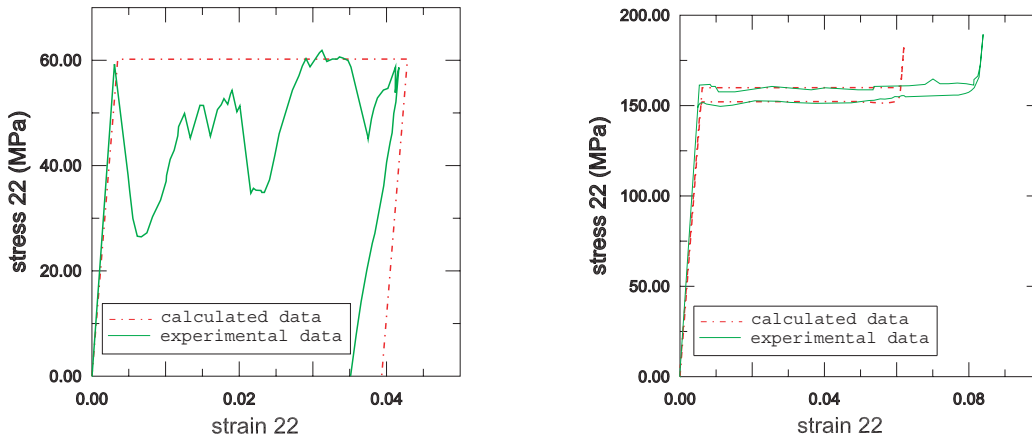


Figure 2: Comparison of experimental and calculated data, left (a) for SME-specimen, and right (b) for SE-specimen

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