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A MICROMECHANICAL MODEL FOR SINGLE-CRYSTAL SHAPE-MEMORY-ALLOYS

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Summary This work is dealing with solid to solid phase transformations in shape-memory-alloys and the simulation of the characteristic phenomena, e.g. pseudoelasticity and the shape-memory-effect. In particular it focuses on the micromechanical behaviour of the material like the appearance of microstructures.

The mechanical model is based on the idea of combining energy densities of several martensite and one austenite phase to an averaged energy density of the mixture within a representative volume element (RVE). Let us assume that we want to simulate the behaviour of shape-memory-alloys like Indium-Thallium (InTl), which undergo a cubic to tetragonal transformation. According to [1] we have to take 3 martensite variants in account.
The averaged energy density of the representative volume element can be written as

$$\bar{\psi} = \left(1 - \sum_{i=1}^{3} \beta_i\right) W_A(\boldsymbol{\varepsilon}) + \sum_{i=1}^{3} \beta_i \, W_{M_i}(\boldsymbol{\varepsilon}) \tag{1}$$

where W_A is the free energy of the austenite phase and W_{M_i} is the free energy of the martensite variant i. The phase-energies are adopted from a thermomechanical approach by Frémond [3] and consist only of physically well defined properties, e.g. the fourth-order isotropic material tensor or the heat-expansion-coefficient. The symbols β_i represent the volume fraction of the martensite variant i and can be treated as internal variables from the mechanical point of view.
Regarding all β_i as minimizers of the energy functional will lead us to a non-quasiconvex problem as shown in [4]. This can be avoided by the assumption of an inhomogenous distribution of the strain $\boldsymbol{\varepsilon}$ which constitutes a microstructure. We assume a certain microstructure which is inspired by those found in micrographs [2] as shown in fig.1(left). It consists of

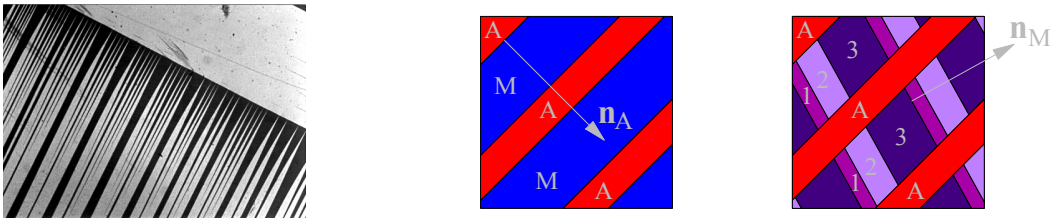

Figure 1. micrograph of martensite twins (left) and assumed microstructure (right)

alternating regions of austenite and martensite, which are repeated periodically. These regions, which are called laminates, are orientated along a direction $\mathbf{n}_A$. The martensite-laminate itself consists of the three different variants, which are supposed to be arranged in laminates too and orientated along a different direction n_M (see fig.1,right). We assume deformation-states in the different laminates, which are compatible at the interfacial boundaries and, integrated over the whole RVE, equivalent to the homogenous macroscopic deformations, as follows:

$$\boldsymbol{\varepsilon}_A \;:=\; \boldsymbol{\varepsilon} - \left(\sum_{i=1}^{3} \beta_i\right) (\mathbf{u}_A \otimes_s \mathbf{n}_A) \tag{2}$$

$$\boldsymbol{\varepsilon}_i \;:=\; \begin{cases} \boldsymbol{\varepsilon} + \left(1 - \sum\limits_{i=1}^{3} \beta_i\right) (\mathbf{u}_A \otimes_s \mathbf{n}_A) + \beta_3 \, (\mathbf{u}_i \otimes_s \mathbf{n}_M)\,, & \text{if } i = 1 \ldots 2 \\ \boldsymbol{\varepsilon} + \left(1 - \sum\limits_{i=1}^{3} \beta_i\right) (\mathbf{u}_A \otimes_s \mathbf{n}_A) - \sum\limits_{j=1}^{2} \beta_j \, (\mathbf{u}_j \otimes_s \mathbf{n}_M) & , \text{ if } i = 3 \end{cases} \tag{3}$$

with $\mathbf{u}_A \otimes_s \mathbf{n}_A := \mathbf{u}_A \otimes \mathbf{n}_A + \mathbf{n}_A \otimes \mathbf{u}_A$. The averaged energy density can now be written as

$$\bar{\psi} = \left(1 - \sum_{i=1}^{3} \beta_i\right) W_A(\boldsymbol{\varepsilon}_A) + \sum_{i=1}^{3} \beta_i \, W_{M_i}(\boldsymbol{\varepsilon}_i) \qquad . \tag{4}$$

The variables $\mathbf{u}_A$,$\mathbf{u}_1$,$\mathbf{u}_2$ are considered as minimizers of the averaged energy density. This minimization process yields the relaxed energy functional

$$\psi R_1 = W_A(\boldsymbol{\varepsilon}) + \sum_{i=1}^{3} \beta_i \, c - \alpha \, \bar{\boldsymbol{\tau}} : \boldsymbol{\varepsilon} + \mathcal{G}_{R_1}\left(\boldsymbol{\beta}, \mathbf{n}_A, \mathbf{n}_M\right) \tag{5}$$

with

$$\mathcal{G}_{R_1}\left(\boldsymbol{\beta}, \mathbf{n}_A, \mathbf{n}_M\right) = -\alpha \left[\left(1 - \sum_i \beta_i\right) \mathbf{u}_A \cdot \bar{\boldsymbol{\tau}} \cdot \mathbf{n}_A + \beta_1 \, \beta_3 \, \mathbf{u}_1 \cdot (\boldsymbol{\tau}_1 - \boldsymbol{\tau}_3) \cdot \mathbf{n}_M + \beta_2 \, \beta_3 \, \mathbf{u}_2 \cdot (\boldsymbol{\tau}_2 - \boldsymbol{\tau}_3) \cdot \mathbf{n}_M \right] \tag{6}$$

The remaining variables are related to dissipative energy terms. We can derive evolution equations from a given dissipation functional $\Delta(\dot{\mathbf{P}})$, where the vector $\mathbf{P}$ contains all remaining variables. The minimization of the total power expended in the material leads us to the condition

$$\dot{\mathbf{P}} \in \frac{\partial J(\mathbf{Q})}{\partial \mathbf{Q}} \tag{7}$$

with the Legendre-transform of $\Delta(\dot{\mathbf{P}})$

$$J\left(\mathbf{Q}\right) := \max\left\{\mathbf{Q} \cdot \dot{\mathbf{P}} - \Delta; \dot{\mathbf{P}}\right\} \tag{8}$$

and

$$Q_i := -\frac{\partial \psi R_1}{\partial P_i} \quad , i = 1 \ldots 9 \qquad . \tag{9}$$

We are now able to simulate the characteristic hysteretic behaviour of shape-memory-alloys. Fig.2 shows the results of a homogenous uni-axial tension-test.

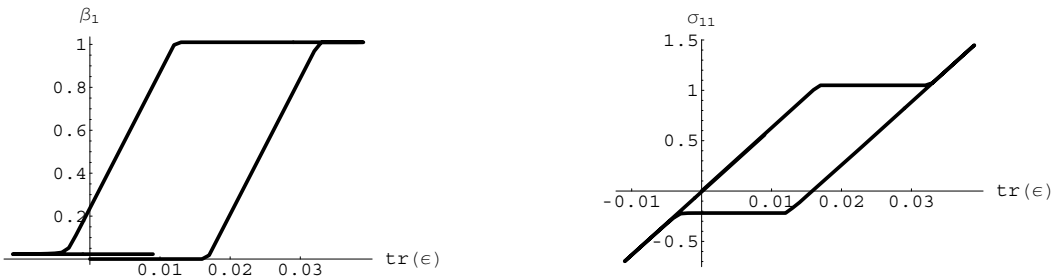

Figure 2. results for the volume fraction β_1 and the stress component σ_{11}

For the analysis of structures we can apply the introduced algorithm to the FEM, where the local computation mentioned above is done at every Gauss-Point. Fig.3 shows the results of a bending test of a 2D-structure.

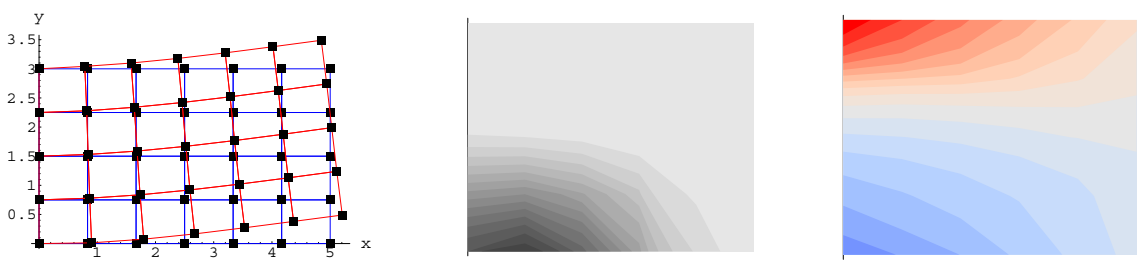

Figure 3. results for the volume fraction β_1 and the stress component σ_{11}

References

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