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Modeling and simulation of phase transformations in polycrystals – a micro-sphere framework

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Micro Abstract
A new framework for the simulation of shape memory alloys (SMA) and TRIP steels undergoing martensite-austenite phase transformations is introduced. The goal is the derivation and elaboration of a generalised model which facilitates the reflection of the characteristic macroscopic behaviour of SMA as well as of TRIP steels. The model is implemented in a micro-sphere formulation in order to capture polycrystalline behaviour and to simulate three-dimensional boundary value problems.

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Introduction

The micro-sphere framework is a powerful tool for the modeling of different phenomena observed in different classes of solids, cf., e.g., [3–5, 9] for the micro-sphere-based modelling of dissipative and non-dissipative effects in rubber, bone, and polycrystalline metals. As a basis for the material model presented here—aiming at the simulation of polycrystalline materials undergoing solid to solid phase transformations—we introduce a formulation where a Helmholtz free energy function depending on volumetric and deviatoric strain measures—as well as plastic strains and temperature—is assigned to each phase. A Legendre transformation of the potential yields the overall Gibbs energy density, based on which we calculate Gibbs energy barriers, cf. [6]. The energy barriers enter a transformation approach derived from statistical physics, enabling the specification of evolution equations for individual volume fractions. The resulting formulation is embedded in a micro-sphere framework for the simulation of three-dimensional boundary value problems. Within the finite element implementation, the local material behaviour in each integration point is governed by an individual response of the micro-sphere model.

1 Infinitesimal strain formulation

For all phases $\alpha \in \{1, \dots, \nu\} \subset \mathbb{N}$ within the multi-phase formulation, the corresponding volume fractions $\xi^\alpha \in [0,1] \subset \mathbb{R}$ are subject to $\sum_\alpha \xi^\alpha = 1$, so that $\sum_\alpha \dot{\xi}^\alpha = 0$, as implied by mass conservation. The evolution of the individual volume fractions ξ^α is based on an approach from statistical physics, where a transformation probability matrix—or rather the infinitesimal generator of a Markov process—$\boldsymbol{Q} \in \mathbb{R}^{\nu \times \nu}$ drives the phase evolution via $\dot{\boldsymbol{\xi}} = \boldsymbol{Q} \cdot \boldsymbol{\xi}$, cf. [2]. The operator $\boldsymbol{Q}$ is composed of transformation probabilites $P_{\alpha \to \beta} \in [0,1] \subset \mathbb{R}$, which themselves are derived from Gibbs energy barriers $b_{\alpha \to \beta}$ that need to be overcome for transformation from one phase, say α, to another phase, say β.

The overall Helmholtz free energy potential of the phase mixture is denoted as $\Psi = \sum_\alpha \xi^\alpha \psi^\alpha$, with $\psi^\alpha = \widehat{\psi}^\alpha(\varepsilon_{\text{dev}}, \varepsilon_{\text{vol}}, \varepsilon^\alpha_{\text{pl}}, \theta)$ the Helmholtz free energy associated to any given phase α depending on a deviatoric and volumetric strain measure, ε_{dev} and ε_{vol}, as well as plastic

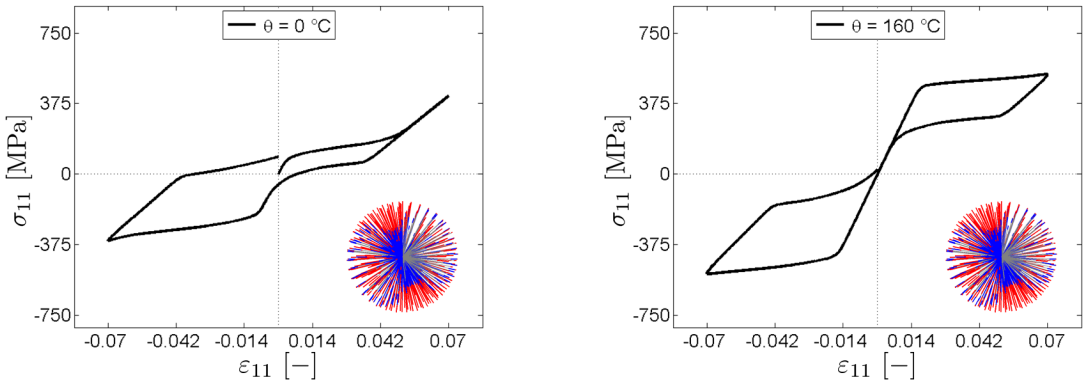

Figure 1. Temperature-dependent response obtained for a SMA simulation within the infinitesimal strain framework: the formulation captures the pseudo-plastic behaviour at lower temperatures, such as $\theta = 0\,^{\circ}\mathrm{C}$ (left), as well as the pseudo-elastic behaviour typically observed at elevated temperatures ($\theta = 160\,^{\circ}\mathrm{C}$, right).

strains $\varepsilon^{\alpha}_{\mathrm{pl}}$ and temperature θ. In view of the embedding into a micro-sphere framework with volumetric-deviatoric split in kinematics, the individual energy contributions are composed of deviatoric and volumetric energy terms, $\psi^{\alpha}_{\mathrm{dev}}$ and $\psi^{\alpha}_{\mathrm{vol}}$, besides thermal and chemical parts, so that $\psi^{\alpha} = \psi^{\alpha}_{\mathrm{dev}} + \psi^{\alpha}_{\mathrm{vol}} + \psi^{\alpha}_{\mathrm{therm}} + \psi^{\alpha}_{\mathrm{chem}}$. Details on the specification of these terms are provided in [7].

1.1 Macroscopic stress response and tangent operator

In the context of the infinitesimal strain micro-sphere approach, the macroscopic stress tensor $\boldsymbol{\sigma}$ is obtained by integration over the unit sphere, resulting in the numerical approximation

$$\boldsymbol{\sigma} = \frac{1}{4\,\pi}\int_{\mathbb{U}^2}\frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}}\,\mathrm{d}a \approx \sum_{i=1}^{n_r}\frac{\partial \Psi_i}{\partial \boldsymbol{\varepsilon}}\,\bar{w}_i = \sum_{i=1}^{n_r}\frac{\partial}{\partial \boldsymbol{\varepsilon}}\left(\sum_{\alpha=1}^{\nu}\xi^{\alpha}_i\psi^{\alpha}_i\right)\bar{w}_i = \sum_{i=1}^{n_r}\sum_{\alpha=1}^{\nu}\xi^{\alpha}_i\boldsymbol{\sigma}^{\alpha}_i \tag{1}$$

with $\boldsymbol{\sigma}^{\alpha}_i$ the tensor-valued stress contribution of phase α situated in the ith micro-sphere integration direction and n_r the number of spatial integration directions. A representative stress-strain response obtained for SMA at different temperature levels is provided in Fig. 1. In view of the finite element implementation, the required algorithmic tangent modulus reads

$$\mathbf{E}^{\mathrm{alg}} := \frac{\mathrm{d}\boldsymbol{\sigma}}{\mathrm{d}\boldsymbol{\varepsilon}} = \sum_{i=1}^{n_r}\frac{\partial \boldsymbol{\sigma}_i}{\partial \boldsymbol{\varepsilon}} + \sum_{i=1}^{n_r}\sum_{\alpha=1}^{\nu}\frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{s}^{\alpha}_i}\cdot\frac{\partial \boldsymbol{s}^{\alpha}_i}{\partial \boldsymbol{\varepsilon}}\,, \tag{2}$$

with $\boldsymbol{s}^{\alpha}_i = [\xi^{\alpha}_i, \varepsilon^{\alpha}_{\mathrm{pl},i}]$ the vector of internal variables associated to phase α in the ith micro-sphere integration direction $\boldsymbol{r}_i$. To highlight the behaviour of the model under inhomogeneous loads, we provide the results of a finite element simulation in Fig. 2.

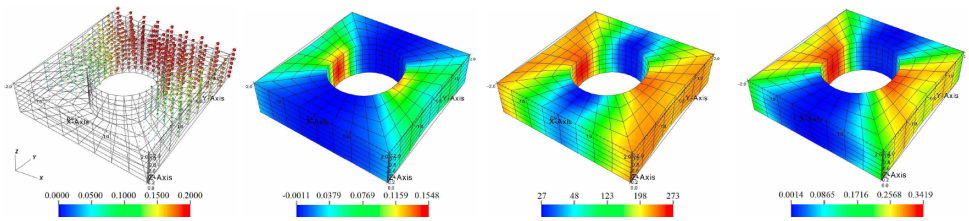

Figure 2. Finite element implementation of the infinitesimal strain micro-sphere formulation: prescribed tensile displacements, tensile strains, tensile stresses, evolution of martensite (from left to right), cf. [5].

2 Finite strain extension

The aforementioned formulation, introduced within an infinitesimal strain micro-sphere framework, captures several experimentally observed effects of SMA and TRIP steel undergoing phase

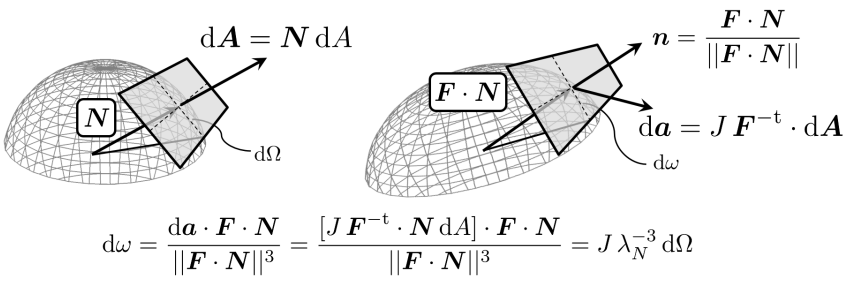

Figure 3. Differential geometric relations for the finite strain micro-sphere framework.

transformations—including the temperature-dependent pseudo-elastic and pseudo-plastic behaviour of SMA, the stress-strain-temperature response of SMA, and the macroscopic stress-strain response including work hardening of TRIP steel [5]. We now aim at the finite strain generalisation of the overall formulation. For conceptual clarity, we restrict this extension to an austenitic parent phase, A, and a single martensitic tensile phase, M, for now, i.e. $\alpha = \{\mathrm{A}, \mathrm{M}\}$. Moreover, we consider only one kinematic strain measure, the normal strain λ_N, on the micro-plane. Following the thermodynamically consistent finite strain micro-sphere framework established in [1], this strain is characterised as $\lambda_N = ||\boldsymbol{F}\cdot\boldsymbol{N}|| = \sqrt{\boldsymbol{N}\cdot\boldsymbol{C}\cdot\boldsymbol{N}}$ with $\boldsymbol{N}$ the normal of the associated material micro-plane, cf. Fig. 3.

2.1 Multiplicative strain decomposition and free energy

In view of Bain-type transformation strains associated with the martensite phase, the micro-plane strain measure is multiplicatively decomposed into elastic and transformation related contributions, λ_N^α and $\lambda_{\mathrm{tr}}^\alpha$, via $\lambda_N = \lambda_N^\alpha\,\lambda_{\mathrm{tr}}^\alpha$. The elastic strains entering the free energy function of a particular phase, say α, thus directly follow as $\lambda_N^\alpha = \lambda_N\,[\lambda_{\mathrm{tr}}^\alpha]^{-1}$. Here, the index N relates to the micro-sphere integration direction with material normal $\boldsymbol{N}$, cf. Fig. 3.

The micro-plane Helmholtz free energy $\psi_N^\alpha = \widehat{\psi}_N^\alpha(\lambda_N)$ for each phase α is chosen as

$$\widehat{\psi}_N^\alpha(\lambda_N) = \mathsf{E}^\alpha \left[\frac{1}{2}\left[\lambda_N\,[\lambda_{\mathrm{tr}}^\alpha]^{-1}\right]^2 + \frac{1}{3}\left[\lambda_N\,[\lambda_{\mathrm{tr}}^\alpha]^{-1}\right]^{-3} - \frac{5}{6}\right] , \tag{3}$$

with E^α representing a scalar-valued micro-plane elasticity coefficent. This specific energy potential is a straight-forward extension of the structure elaborated in [1]. The overall Helmholtz free energy $\Psi_N = \widehat{\Psi}_N(\lambda_N)$ of the phase mixture associated to the micro-plane with material normal $\boldsymbol{N}$ is $\widehat{\Psi}_N(\lambda_N) = \sum_\alpha \xi_N^\alpha\,\widehat{\psi}_N^\alpha(\lambda_N)$.

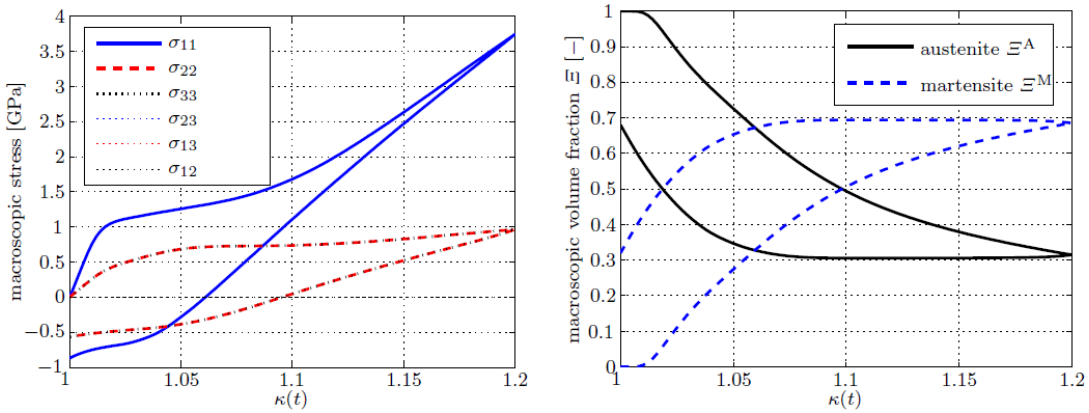

Figure 4. Macroscopic stress-strain response (left) and naturally captured grain locking effect (right). $\boldsymbol{F}(t) = \boldsymbol{I} + \kappa(t)\,\boldsymbol{e}_1 \otimes \boldsymbol{e}_1$ with $\kappa(t) \in [0, 0.2] \subset \mathbb{R}$ is prescribed as a time-proportional load, cf. [8].

2.2 Macroscopic stress response

The material stress $S_N = \widehat{S}_N(\lambda_N)$ associated with a micro-plane N follows from (3) via $\widehat{S}_N(\lambda_N) = \partial\widehat{\Psi}_N(\lambda_N)/\partial\lambda_N = \sum_\alpha \xi_N^\alpha \, \partial\widehat{\psi}_N^\alpha(\lambda_N)/\partial\lambda_N$. The macroscopic Cauchy stress tensor $\boldsymbol{\sigma}$ then reads

$$\boldsymbol{\sigma} = \frac{1}{J}\,\boldsymbol{F}\cdot\left[\frac{3}{4\,\pi}\int_{\mathbb{U}^2}\widehat{S}(\lambda_N)\,\lambda_N^{-1}\,\boldsymbol{N}\otimes\boldsymbol{N}\,\mathrm{d}\omega\right]\cdot\boldsymbol{F}^{\mathrm{t}}\ , \tag{4}$$

with an exemplary, representative computation provided in Fig. 4.

Conclusions

For the formulation of a model that captures the austenitic-martensitic tranformation behaviour both in shape memory alloys (SMA) and in TRIP steels, a couple of aspects need careful attention. In TRIP steels, the interactions between plasticity and phase transformations play an important role in view of the overall macroscopic response. As a result, appropriate models need to take into account multi-phase plasticity. Moreover, the experimentally observed volume change that TRIP steel, unlike SMA, shows during ongoing phase transitions must be accounted for. To this end, the framework presented here—formulated in terms of decoupled deviatoric and volumetric strain measures—facilitates introducing a non-zero volumetric transformation strain, cf. [7]. Finally, appropriate hardening laws are required to capture the pronounced work hardening related to TRIP steel, cf. [5].

The provided ansatz for a generalisation of the infinitesimal strain framework towards a geometrically exact formulation is viewed as a promising foundation for further extensions towards coupled anisotropic finite strain plasticity and temperature effects in polycrystals undergoing large strains.

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