A VARIATIONAL FRAMEWORK FOR THE MODELLING OF VARIANT SWITCHING AND REORIENTATION IN MSMA USING ENERGY RELAXATION METHODS

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1. Introduction

The aim of this presentation is to emphasize the application of quasiconvex analysis to the modelling and simulation of martensite variant switching and reorientation in ferromagnetic materials. The underlying microstructure is accurately modelled and parametrized and representative results are shown for two specific model problems.

2. Mathematical prerequisites

The term quasiconvexity, as introduced in [1], is a necessary condition for the existence of minimizers of functionals. For application purposes, quasiconvexification, as for example used in [2] among others, aims at the determination of an optimal, since energy minimizing, displacement perturbation field $\boldsymbol{w}$ which then yields the quasiconvex energy hull

$$\psi^{\mathrm{Q}}(\boldsymbol{F}) := \min_{\boldsymbol{w}} \left\{ \int_{\mathcal{B}} \psi(\boldsymbol{F} + \nabla \boldsymbol{w}) \, \mathrm{d}V \right\} \tag{1}$$

This perturbation field can be associated with a specific microstructure of a representative volume element (RVE) at the microscale of the underlying material. This microstructure will be induced in case the energy loses its quasiconvexity and the mixture of different phases thus becomes energetically favorable.

3. Constitutive framework

In this contribution, a variational framework for the modeling of phase-transforming solids including magneto-mechanical coupling using energy relaxation methods is shown. The point of departure is an energy functional $\Pi(\boldsymbol{u},\phi,\boldsymbol{m})$ depending on the global field variables $\boldsymbol{u}$ as the displacement field, ϕ as the magnetic potential, and $\boldsymbol{m}$ as the magnetization. In line with [3], this functional is chosen such that the Euler-Lagrange equations obtained via variational calculus yield the mechanical equilibrium conditions, the Gauß-Faraday law, the respective associated Neumann boundary conditions, and a constitutive relation between the total magnetic field and the magnetization.

In this context, the energy contribution stemming from elastic deformations is generally obtained by a standard mixture rule, which takes into account all relevant phases of the underlying material. For materials such as magnetic shape memory alloys (MSMA), there exist “mechanical phases” in terms of different Bain strains as well as “magnetic phases”, which differ from each other in terms of the direction of spontaneous magnetization. In this regard, the magnetization $\boldsymbol{m}$ is treated as a function depending on the volume fractions of the respective phases and the associated spontaneous magnetizations.

With these prerequisites at hand, the perturbation field introduced in (1) is parametrized via generalized internal variables $\boldsymbol{p}$ such that the relaxed energy density (as an approximation of the quasiconvex energy density) is defined as

$$\psi^{\mathrm{rel}}(\boldsymbol{F}) := \min_{\boldsymbol{p}} \left\{ \int_{\mathcal{B}} \psi(\boldsymbol{F} + \nabla \boldsymbol{w}(\boldsymbol{p}))\, \mathrm{d}V \right\} \tag{2}$$

This minimization procedure yields the optimal arrangement of phases in terms of orientations and volume fractions and defines the effective material response, e.g., with respect to stresses.

4. Incremental variational principle

As indicated above, the solution of the problem at hand is based on the definition of an energy potential precisely given by

$$\Pi(\boldsymbol{\varepsilon}) := V_{\mathcal{B}} \left[\psi^{\mathrm{rel}} + \frac{\mu_0}{2} \boldsymbol{m} \cdot \mathbf{D} \cdot \boldsymbol{m} - \mu_0 \, \overline{\boldsymbol{h}} \cdot \boldsymbol{m} - \overline{\boldsymbol{\sigma}} : \boldsymbol{\varepsilon} \right] \tag{3}$$

Here, a homogeneously distributed magnetic field and stress field is assumed, where the demagnetization field can be represented by the demagnetization tensor $\mathbf{D}$. The elastic part of the energy is defined by the relaxed energy density defined in (2). In line with, e.g., [3], this energy is embedded into an incremental minimization principle where dissipation is accounted for in terms of a dissipation functional depending on the rates of dissipative internal state variables. The stationary point of this total incremental energy functional then yields the optimal values for all state dependent variables.

5. Numerical examples: Application to two model problems

For the numerical examples shown in the presentation, the theoretical framework is applied to two specific model problems: variant switching (between different martensite variants) and reorientation in MSMA as well as phase transitions between austenite and several martensite phases in conventional SMA. In the context of the first model problem it is shown, that the framework is capable of reproducing physically sound results in comparison with experimental findings. The main aim with respect to the second model is the establishment of an enhanced energy relaxation scheme for single-crystalline materials subjected to phase transformations.

6. References

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