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Multiscale FE-FFT-based thermo-mechanically coupled modeling of viscoplastic polycrystalline materials

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Micro Abstract
A two-scale finite element (FE) and fast Fourier transform (FFT) based thermo-mechanically coupled model is proposed. The method is developed for the prediction of the structural material behavior and the corresponding local fields of elasto-viscoplastic polycrystalline materials. It allows for a qualitative investigation of the microscopic interplay between stress and temperature induced martensitic phase transformation and plasticity.

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Introduction

Polycrystalline materials (e.g. steels) have superior mechanical properties and are thus important for numerous technically relevant applications. The prediction of the effective behavior of these materials represents an enormous challenge. This is due to the fact that the distribution, morphology and orientation of individual grains on the microscopic level strongly influence the macroscopic structural response. In addition, complex interactions between different deformation mechanisms (e.g. plastic slip and martensitic phase transformation) on the micro scale can occur and affect the mechanical behavior. As a consequence, two different continuum scales need to be studied in order to capture the microstructural influence on structural finite element (FE) simulations. Recently, [6] and [3] published finite element and fast Fourier transform (FFT) based methods to predict the local and effective mechanical response of heterogeneous materials. Compared to the classical multiscale finite element or FE^2 method this approach exhibits significant advantages with respect to computational efficiency [5].
In this work a two-scale FE-FFT based and thermo-mechanically coupled material model formulation for elasto-viscoplastic polycrystalline materials is developed. Temperature and stress induced martensitic phase transformations are considered. Following [1], a meso-scale description of the crystal configurations, based on the volume fractions λ_i of the different martensite variants, is derived. The direction of plastic dislocation motion is prescribed by up to 48 different slip systems and depending on the crystal system and grain orientation. The evolution of plastic slip is modeled by means of a power law based flow rule in accordance with [4].

1 Material model

To solve the thermo-mechanically coupled multiscale problem it is essential to fulfill the mechanical equilibrium (2) and energy balance (3) at both scales. In what follows, macroscopic quantities are denoted by the subscript M and microscopic fields by no index to distinguish between the two scales.
The macroscopic boundary value problem is solved by employing the finite element method. The microscopic structure is embedded at the Gauss-points of each element, to deduce the form of the constitutive relation between macroscopic strain $\boldsymbol{\varepsilon}_M$ and stress $\boldsymbol{\sigma}_M$ and further the

macroscopic internal heat sources r_M. To this end the macroscopic strain and temperature θ_M are transferred to the microscale, during the FE solution procedure. The unknown macroscopic quantities ($\boldsymbol{\sigma}_M$, r_M) are subsequently determined by finding the solution of the local problem and are obtained from homogenization of the corresponding micro-scale quantities. Figure 1 gives an overview of the proposed scale transition and solution method.

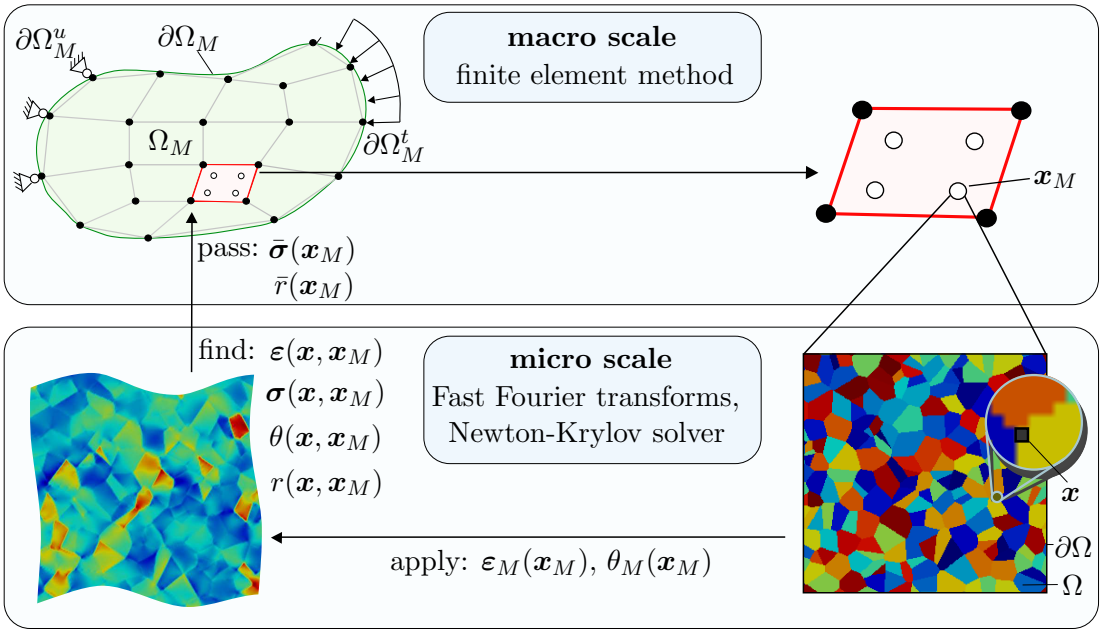

Figure 1. Overview of proposed scale transition and solution method

The microstructure is embedded as a unit cell of the domain Ω at each $\boldsymbol{x}_M \in \Omega_M$ with periodic boundary conditions. To solve the local problem we additively decompose the total microscopic strain

$$\boldsymbol{\varepsilon}(\boldsymbol{x}, \boldsymbol{x}_M) = \bar{\boldsymbol{\varepsilon}}(\boldsymbol{x}_M) + \tilde{\boldsymbol{\varepsilon}}(\boldsymbol{x}) \tag{1}$$

into the mean strain $\bar{\boldsymbol{\varepsilon}}$ and the local fluctuation $\tilde{\boldsymbol{\varepsilon}}$. The homogeneous contribution $\bar{\boldsymbol{\varepsilon}}$ is equal to the macroscopic strain $\boldsymbol{\varepsilon}_M$ and therefore independent of $\boldsymbol{x} \in \Omega$. Thus, using FFT-based solution schemes the local strain fluctuation around the mean strain represents the primary unknown of the local, nonlinear mechanical equilibrium condition.

$$\operatorname{div}(\boldsymbol{\sigma}(\boldsymbol{x}, \varepsilon, \theta, \boldsymbol{\xi})) = \mathbf{0} \qquad \text{for } \boldsymbol{x} \in \Omega \tag{2}$$

In addition $\boldsymbol{\xi}$ is a set of local internal variables representing plastic slip and martensitic phase transformation.

The time- and length-scale of the underlying unit cell can be assumed much smaller than their counterparts in the macro-scale. We therefore presume that macroscopic temperature changes affect the temperature at each point of the micro structure instantaneously and simultaneously. Consequently, the macroscopic temperature will be represented as a steady state, homogeneous temperature field on the micro scale.

However, dissipative effects on the micro scale due to plasticity and phase transformation should not be neglected throughout this work. Hence the local temperature field is divided conceptually into the homogeneous macroscopic temperature contribution θ_M and a transient heterogeneous field θ_L. Based on the previous considerations, we only need to pass the macroscopic temperature and not its gradient to the unit cell, to solve the local reduced energy equilibrium:

$$\rho C_v \dot{\theta}(\boldsymbol{x}) = \rho C_v (\underbrace{\dot{\theta}_M}_{\approx 0} + \dot{\theta}_L(\boldsymbol{x})) = r(\boldsymbol{x}, \varepsilon, \theta, \boldsymbol{\xi})) - \operatorname{div}(\boldsymbol{q}(\boldsymbol{x}, \theta)) \qquad \text{for } \boldsymbol{x} \in \Omega \tag{3}$$

Here, C_v is the heat capacity storage, ρ denotes the density and $\boldsymbol{q}$ represents the heat flux vector.

We postulate an additive decomposition of the Helmholtz free energy

$$\Psi(\boldsymbol{\varepsilon}, \boldsymbol{\gamma}, \boldsymbol{\lambda}, \theta, \boldsymbol{x}) = \Psi^e(\boldsymbol{\varepsilon}, \boldsymbol{\gamma}, \boldsymbol{\lambda}, \theta) + \Psi^p(\boldsymbol{\gamma}, \theta) + \Psi^t(\boldsymbol{\lambda}, \theta) + \Psi^\theta(\theta) \tag{4}$$

,where Ψ^e is the elastic energy density. The stored energy due to plastic work is represented by Ψ^p and depends on the slip $\boldsymbol{\gamma} = \{\gamma_\alpha\}$ on each slip system α and the temperature. The energy associated with martensitic transformation Ψ^t is a function of $\boldsymbol{\lambda} = \{\lambda_i\}$ the volume fraction of all martensite variants λ_i and the temperature. The thermal energy density is Ψ^θ. The stress and entropy η are governed by

$$\boldsymbol{\sigma} = \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}}, \qquad \eta = -\frac{\partial \Psi}{\partial \theta} \tag{5}$$

and the evolution equations of the internal variables

$$\dot{\lambda}_i = f_i\left(-\frac{\partial \Psi}{\partial \lambda_i}, \theta\right), \qquad \dot{\gamma}_\alpha = g_\alpha\left(-\frac{\partial \Psi}{\partial \gamma_\alpha}, \theta\right) \tag{6}$$

are functions of the associated driving forces and the temperature. In accordance with [4] the evolution of the plastic strain is obtained by a power law based flow rule being solved by an algorithm proposed by [7]. Following [1] a kinetic potential is introduced to determine the evolution of transformation.

The computational solution procedure for the local problem is based on fast Fourier transforms and Newton-Krylov methods and a staggered implicit time integration scheme is applied. To this end, the local mechanical boundary value problem is solved first. In a staggered update, the heterogeneous temperature field and martensitic phase evolution of the underlying unit cell is determined. The components of the global algorithmic tangent are calculated numerically by finite differences, which requires a repeated performance of the microscopic solution procedure.

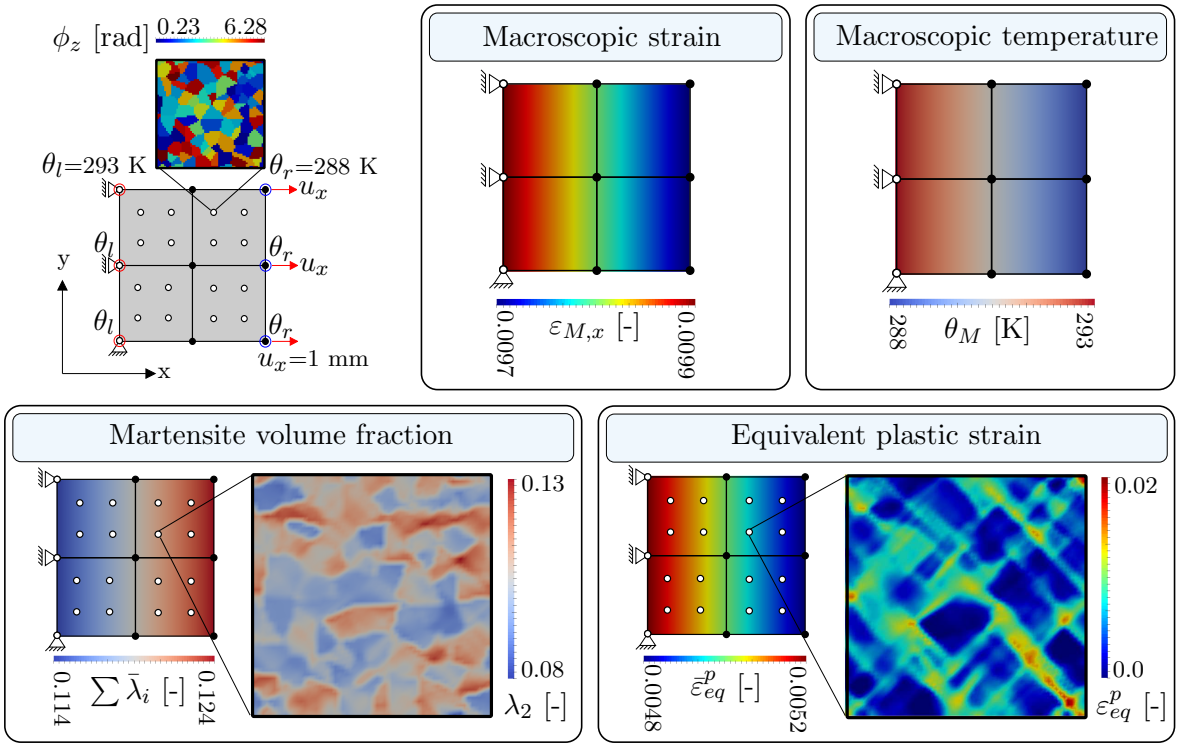

Figure 2. Macro- and microscopic results for thermo-mechanical loading conditions

2 Computational example

We study a simple virtual experiment to provide an insight into the capabilities of the model. The proposed formulation is implemented as an extension to the finite element software FEAP. A plane strain example is considered. At each Gauss-point of the fully integrated, 8-node, cubic finite elements a polycrystalline micro structure is embedded. The latter is composed of 100 grains with random orientation ϕ_z. In figure 2 the thermo-mechanical loading and boundary conditions as well as the results for this loading sequence are displayed for selected fields on the macro (finite element model) and on the micro scale (unit cell).
Considering macroscopic steady state temperature conditions, we obtain a constant, macroscopic temperature gradient in x-direction (see figure 2). Hence, the primarily temperature induced evolution of martensite is distributed heterogeneously on the macro scale . On the micro scale a complex interplay between plasticity and transformation arises. Plastic deformations are initiated in grains that are oriented poorly for transformation and provide a bridge across less transformed regions. All these results are qualitatively consistent with experimental observation and the prediction of e.g. [2] and [1].

Conclusions

The proposed FE-FFT-based method represents an efficient and novel tool to predict the local and structural response of polycrystalline materials under thermo-mechanical loading conditions. The model allows for various further investigations of the interplay between crystal plasticity, martensitic transformation and the corresponding dissipative effects.

Acknowledgements

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