

Shape memory alloys (SMA) exhibit unusual properties such as shape recovery and pseudoelasticity which are due to reversible martensitic phase transformation. Martensitic transformation can be induced by mechanical loading or by varying temperature, and it proceeds by formation and evolution of complex microstructures. Modelling of microstructure evolution is essential for understanding and predicting material behaviour at the micro-scale.

Unusual properties of SMA make them attractive materials for numerous applications in engineering and medicine, and some of them have already been implemented in practice. Reliable and computationally efficient models are thus obviously needed both at the micro- and macro-scale. The goal of micro-scale modelling is to provide insight into the microscopic deformation mechanisms and to support development of improved materials, for instance, with enhanced resistance to structural and functional fatigue. Results of micromechanical modelling can also be used to formulate and calibrate macroscopic models. The macroscopic models are needed, for instance, to support development and optimization of SMA devices.

The phase-field method is an efficient tool for modelling of phase transformations and the related microstructure evolution. The essence of phase-field modelling is in introducing a diffuse-interface approximation of the interphase boundaries. Specifically, a so-called order parameter is introduced which varies continuously between the two states, and intermediate values correspond to a diffuse interface, the properties of which are interpolated between the values corresponding to the pure phases. The main benefit of the diffuse-interface approach is that it leads to efficient computational schemes in which formation and evolution of microstructure can be modelled on a fixed computational mesh (or grid). Tracking of actual interfaces is thus avoided and the interfaces may nucleate, propagate and annihilate independently of the computational mesh.

The aim of the present project is to develop a new phase-field model of evolution of martensitic microstructures. Analysis of the state-of-the-art has revealed that existing models exhibit several deficiencies, and the project aims at developing an improved model that will be free of those deficiencies. This concerns, in particular, one of the basic assumptions adopted in the vast majority of the models, namely that of the simplified linear kinematics within the so-called small-strain theory. At the same time, consideration of the exact geometrically-nonlinear finite-deformation framework introduces important qualitative and quantitative effects, and consistent consideration of those effects in the phase-field modelling framework constitutes an important contribution of the present project. Another novel aspect is enhancing the microstructure evolution law so that it will include effects that have not been considered in the context of phase-field modelling yet (rate-independent dissipation). Such a model is expected to deliver qualitatively different results compared to the existing models.

Computer implementation of the new phase-field model (using the finite element method) and simulations of microstructure evolution in shape memory alloys constitute an important part of the project. Consideration of the innovative aspects discussed above, and also those that are not mentioned in the present short description, will allow us to study effects that could not be tackled using the existing formulations and computational methods used in the context of phase-field modelling.

Computer implementation will be performed using AceGen, an advanced automatic code generation system. AceGen combines the symbolic capabilities of Mathematica with the automatic differentiation (AD) technique and additional tools for optimization of computer codes. The benefit of using AD is that several tedious steps in the traditional computer implementation, such as derivation and coding of the consistent tangent matrix, are automatized. This leads to robust and time-efficient implementation. Also, the resulting computer code is computationally efficient, while exact linearization guarantees optimal quadratic convergence of the Newton method.

Concluding, execution of the planned research tasks will contribute to development of the theory of phase transformations, including the phase-field method (new models and formulations of the phase-field method), to development of computational methods for the phase-field method (new computational algorithms and finite-element implementation), and to progress in the mechanics and micromechanics of martensitic transformations in shape memory alloys (computer simulations and analysis of evolution of martensitic microstructures, including analysis of size effects). The project results will thus advance understanding of the fundamental aspects of martensitic transformations and will advance theoretical and computational tools for the analysis of those phenomena. Accordingly, the planned research is concerned with basic research. While the project is focused on SMA, it is noted that martensitic transformations and related phenomena occur also in other material systems, hence the results of the project may find applications in a more general context.