

Simulation of phase transformations in polycrystalline shape memory alloys using fast Fourier transforms

Johanna Waimann^{1, *}, Christian Gierden² and Stefanie Reese³

Institute of Applied Mechanics, RWTH Aachen University, Mies-van-der-Rohe-Str. 1,
D-52074 Aachen, Germany, www.ifam.rwth-aachen.de

¹johanna.waimann@rwth-aachen.de

²christian.gierden@rwth-aachen.de

³stefanie.reese@rwth-aachen.de

Keywords: microstructure simulation, FFT, shape memory alloys, phase transformation

The microstructural properties of shape memory alloys are mainly influenced by phase transformations between austenite and martensite. Compared to classical steel, not only thermal but also mechanical loads can induce this complex microstructural evolution, see for instance [1]. Compared to a homogenized description of the effect in our earlier works [2] based on variational methods, we now want to show its highly resolved evolution within a polycrystalline microstructure. Therefore, we combine the earlier presented variational approach with the use of fast Fourier transforms (FFT) [3], which enables a localized examination of the phase transformations in the different oriented grains.

The simulation of a highly resolved non-linear material behaviour comes along with a high computational effort. Thus, we additionally apply a model order reduction technique to reduce the computation time. The idea is to use only a reduced number of Fourier modes for the calculations in Fourier space: the considered set of Fourier modes is adapted to the underlying microstructure as presented in [4].

The presentation of the theoretical background as well as of the implemented algorithm is followed by numerical results that underline the performance of our method.

REFERENCES

- [1] M.F.-X. Wagner, Ein Beitrag zur strukturellen und funktionalen Ermüdung von Draehten und Federn aus NiTi-Formgedächtnislegierungen. *Europ. Univ.-Verlag*, 2005.
- [2] J. Waimann, P. Junker and K. Hackl, Modeling the cyclic behaviour of shape memory alloys. *Shap. Mem. Superelasticity*, Vol. **3**, pp. 124–138, 2017.
- [3] H. Moulinec and P. Suquet, A numerical method for computing the overall response of nonlinear composites with complex microstructure. *Comput. Methods Appl. Mech. Eng.*, Vol. **157**(1–2), pp. 69–94, 1998.
- [4] C. Gierden, J. Waimann, B. Svendsen and S. Reese, FFT-based simulation using a reduced set of frequencies adapted to the underlying microstructure. *Comput. Methods Mater. Sci.*, Vol. **21**(1), pp. 51–58, 2021.