Hessisches Kompetenzzentrum
für Hochleistungsrechnen

Multi-Scale Modeling of Additive Manufactured Magnetic Materials

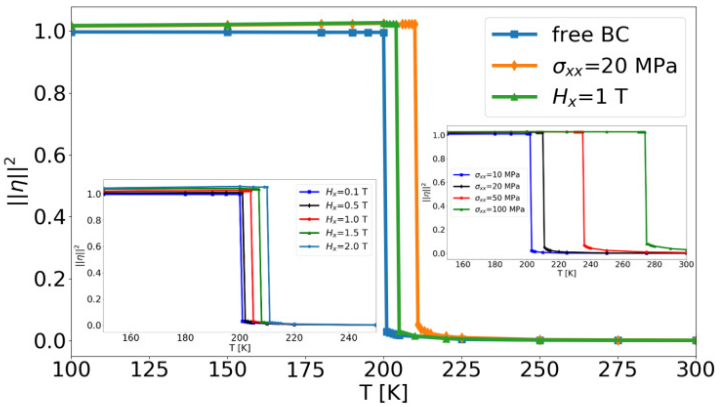


Fig. 1: Evolution of the order parameter ||eta||² as a function of temperature for with and without external stimulus. The right inset shows the shift of transition temperature for different mechanical stress, while the left inset shows the shift for different applied magnetic fields.

Introduction

In 2018, Gottschall et al. proposed a multi-stimulit concept for magnetocaloric cooling. [1] The energy consumption related to cooling is expected to increase significantly over the next decades. Therefore, a more energy efficient and environmental friendly alternative is needed to satisfy the increasing demand. In the multi-stimui concept, the application of magnetic field is complimented with the application of mechanical stress to control the first-order phase transition, e.g. in Heusler alloys. Simulating the multi-stimuli concept using a micromagnetic phase-field model is supposed to support the development of a magnetocaloric cooling device by calculating the potential temperature change ΔT_{ad} within the multi-stimuli concept and for simulation of the heat exchange.

Methods

The Object Oriented MicroMagnetic Framework (OOMMF) code is used to perform purely micromagnetic simulations, utilizing the finite-difference method. For the finite-element implementation of the proposed micromagnetic phase-field model, the open source Multiphysics Object Oriented Simulation Environment (MOOSE) framework is used. Purely mechanical FEM simulations are performed using ABAQUS.

Results

We propose a phase field model based on Landau theory to simulate the magnetic domain evolution during the martensite

Project Manager
Dominik Ohmer

Principal Investigator
Prof. Dr. Bai-Xiang Xu

Project Term
2020 - 2021

Clusters
Lichtenberg Cluster Darmstadt

Software
MATLAB, VASP, OOMMF, Abaqus

Additional Software
MOOSE, Paraview

Institute
FG Mechanik Funktionelle Materialien

University
Technische Universität Darmstadt

JUSTUS-LIEBIG-UNIVERSITÄT GIESSEN
TECHNISCHE UNIVERSITÄT DARMSTADT
UNIKASSEL VERSITÄT
Philipps Universität Marburg

formation in, e.g., Heusler alloys. The model is capable of capturing the magentic martensite transformation, as well as the magnetic martensite to non-magnetic austenite transition. Using temperature-dependent coefficients for the 2-3-4 Landau polynomial and modifying the micromagnetic formulations, the phase transition can be captured. Our proposed model is also capable to capture the shift of the phase transition with applied magnetic field and stress. For the magnetic to non-magnetic transition, we obtain shifts of the transition temperature towards higher temperatures, which is in agreement with experimental results. The application of the external stimuli stabilizes the magnetic martensite phase.

Discussion

The model is shown to be capable of capturing the magnetic martensite state as well as the mangetic martensite to non-magnetic austenite transition. In the martensitic state, the proposed micromagnetic phase-field model is capable of reproducing multi-domain structures with the corresponding magnetic domain microstructure. The transformation of the martensite microstructure with applied stress and magnetic field is captured as well. The three-dimensional, finite-element implementation allows for the investigation of geometry and boundary condition dependent microstructures. In addition to the martensitic state, the modification of the micromagnetic formulations allows for the simulation of the magnetic to non-magnetic phase transition. Application of stress and magnetic field stabilizes the magnetic phase, shifting the transition temperature towards higher temperatures, see Fig. 1.

Publications

Ohmer, D. and Yi, M. and Fries, M. and Gutfleisch, O. and Xu, B. Calculating the magnetocaloric effect in second-order-type material by micromagnetic simulations: A case study on Co2B, Scripta Materialia 177 (2020) 218–222. https://www.doi.org/10.1016/j.scriptamat.2019.10.039

Reference

[1] Gottschall, T., Gràcia-Condal, A., Fries, M. et al. A multicaloric cooling cycle that exploits thermal hysteresis. Nature Mater 17, 929–934 (2018). https://doi.org/10.1038/s41563-018-0166-6

Last Update: 2021-04-14 11:10