Hessisches Kompetenzzentrum
für Hochleistungsrechnen

Multi-Scale Modeling of Additive Manufactured Magnetic Materials

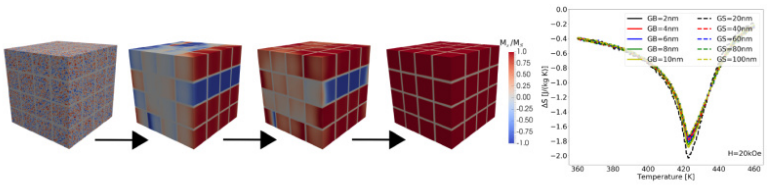

Figure 1: Magnetization reversal process under external magnetic field along the x-axis in Co_2B and specific isothermal entropy change Δ\DeltaS$_T$ calculated via the ANE as a function of grain size and grain boundary thickness. The inset shows the experimentally measured entropy change.

Introduction

In need for alternatives to conventional cooling devices, the magnetocaloric effect (MCE) is one of the most promising candidates for reducing environmentally harmful cooling fluids and increasing the efficiency of cooling devices. The MCE is based on the entropy change of a material during magnetization and demagnetization and therefore depends on the microstructure of the corresponding material. In the framework of the ERC-project ”CoolInnov”, we work together with experimentalists to optimize the microstructure in order to maximize the temperature change during magnetization. Further, a multi-stimuli approach is investigated to combine magnetic fields with pressure to develop a cooling cycle suitable for application in refrigerators. Phase field models are developed to describe the MCE and the influence of pressure and calculated for different microstructures.

Methods

The simulations range from the atomic to the macroscopic scale. On the atomic level, density functional theory (DFT) calculations are performed using the Vienna ab initio Simulation Package (VASP) in order to obtain the magnetocrystalline anisotropy K, saturation magnetization MS, and exchange constant A. The intrinsic magnetic constants are then used to perform micromagnetic simulations using the Object Oriented MicroMagnetic Framework (OOMMF) code to optimize magnetic microstructures. In order to simulate the phase evolution under applied magnetic field or pressure and thus the MCE, finite element method (FEM) simulations are performed on a macroscopic level using the MOOSE (Multiphysics Object Oriented Simulation Environment) framework.

Results

We developed an approach to calculate the MCE based on micromagnetic simulations. Micromagnetic simulations are

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Clusters
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Software
MATLAB, VASP

Additional Software
MOOSE, Paraview

Institute
FG Mechanik Funktionelle Materialien

University
Technische Universität Darmstadt

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restricted to temperatures below the Curie temperature, as the saturation magnetization above Curie temperature is zero. However, application of magnetic fields induce magnetic fields within materials also above Curie temperature. This behavior is not covered by the formalism of micromagnetics. In order to investigate the influence of the microstructure on the MCE, we combined micromagnetic simulations with the phenomenological Arrott-Noakes equation. Numerical paramters required in the Arrott-Noakes equation are obtained for different microstructures using the Kouvel-Fisher method. Using the Arrott-Noakes equation, the entropy change ΔS can be calculated as a function of temperature and the applied magnetic field. Our results show good agreement with measured Co_2B samples.

Discussion

Despite combining micromagnetic simulations and a phenomenological equation for calculating the MCE, our results are in good agreement with experimental results. However, rather than calculating exact values of the MCE properties, our approach is intended to show their tendencies for different microstructures. The methodology introduced can be used to perform a systematic study of the influence of the microstructure on the MCE. In addition, the influence of the magnetic anisotropy K, exchange constant A and saturation magnetization M_S on the MCE can be investigated.

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