Magnetization reversal of large granular magnetic materials

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The simulation size in micromagnetism is typically in the range of nanometers up to a few micrometers depending on the algorithm and availability of computational resources. Computing the hysteresis properties of a magnetic material often requires much larger scales. Solutions to compute spatially restricted areas of EBSD maps in 2D are readily available [1]. In order to simulate the magnetization behavior of full scale EBSD maps, preferably in 3D, the following is required: (A) Stack of EBSD slices of the magnetic material (Figure 1a); (B) Reconstruct the granular structure as finite element mesh by merging slices, smoothing and triangulation of grain boundaries (Figure 1b-d); (C) Computing magnetization reversal of the large structure with conventional micromagnetic solvers or reduced order models.

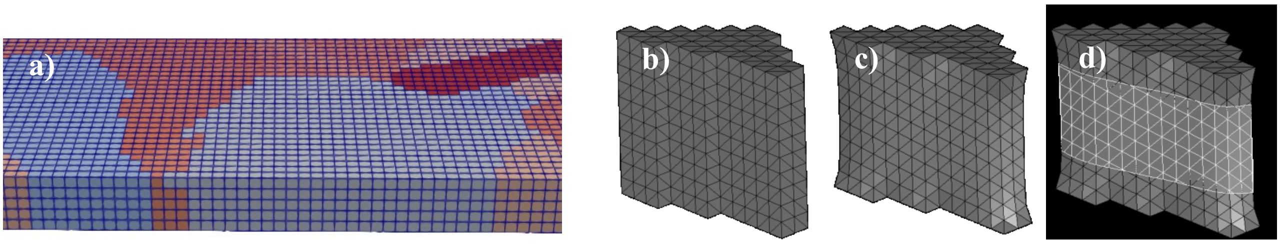

Figure 1: a) Stacked EBSD data of MnAl-C (square edge length 0.3 µm, coloring according to grain orientations), b) Original triangulated grain with square edges, c) laplacian smoothing of grain, d) cutout of final grain.

Although partial solutions are already available, each of the three steps (A to C) is both time-consuming and challenging. In this abstract we will focus mainly on (B), creating the simulation model. Sequential sectioning of the magnetic material in (A) is carried out using a focussed ion beam (FIB) and scanning electron microscope (SEM) at IFW Dresden. A major challenge of the method is the correct angular positioning during measurements, while maintaining accurate overlay of EBSD layers. In (B) a good reconstruction of the grains is achieved by the use of DREAM.3D (dream3d.bluequartz.net, last visited on 2023-03-06). EBSD slices can be imported and merged. A laplacian smoothing filter reduces sharp edges of the original voxel data. Smoothing of the grain boundaries is properly done within the body, but not at the top and bottom (Figure 1c). Postprocessing of the triangulation can be done via Salome (www.salome-platform.org, last visited on 2023-03-06). Unwanted areas at top and bottom can be cut (Figure 1d), yet remeshing of the resulting grains is time-consuming and error prone due to numerical instabilities at, e.g., sharp corners. Directly using the triangulation of DREAM.3D is possible as demagnetization effects of the square edges at the top and bottom may be averaged (Figure 1c). Computation of the hysteresis of the generated structure in C) can be done with conventional micromagnetism in small areas of the EBSD data, similar to [1]. A reduced order model is able to overcome the size limitation. The model is based on the assumption that a nucleation of a sufficiently large reversed domain immediately leads to the magnetic switching of the entire grain in question [2].

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References

[1] M. Gusenbauer, H. Oezelt, J. Fischbacher, A. Kovacs, P. Zhao, T.G. Woodcock, T. Schrefl, Extracting local nucleation fields in permanent magnets using machine learning, npj Computational Materials, 6 (1), 89 (2020)

[2] A. Kovacs, et al. Physics-Informed Machine Learning Combining Experiment and Simulation for the Design of Neodymium-Iron-Boron Permanent Magnets with Reduced Critical-Elements Content, Frontiers in Materials, 9, 1-19 (2023)