Coercivity analysis of twin boundaries with demagnetization negligible models in arbitrary field direction

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Processing of raw materials to develop permanent magnets usually results in crystallographic defects, which can have a significant influence on the coercivity $H_c$ of the magnet, as for instance analyzed in MnAl-C [1]. Tuning the processing routes allows promoting or suppressing certain defects, hence quantifying the influence of the defects is necessary. In this work we demonstrate a simulation procedure, to compute $H_c$ distributions for single defects in arbitrary applied field directions. We use a simple sphere split by a certain defect to avoid demagnetization effects at corners and edges. External field directions are applied evenly distributed around a unit sphere (Fibonacci sphere [2]) pointing to the simulation model in the center (Fig. 1). Each point on the unit sphere corresponds to a micromagnetic simulation, solving the Landau-Lifshitz-Gilbert equation on a tetrahedral finite element grid [3]. The model consists of several segregation layers with varying thickness close to the defect to set different magnetic properties according to measured or estimated material concentrations (Fig. 2).

In MnAl-C twin boundaries have Mn enriched regions at, Mn depleted regions a few nm away, and bulk properties far away from the defect [4,5]. Easy axes configurations are set according to the present twin boundary [5]. Corresponding measurements are performed using sophisticated transmission electron microscopy or atom probe tomography. Using density or distribution plots the trend of different twin configurations can be visualized and compared (Fig. 3). Results show that the coercivity tends to increase with increasing structural and chemical disorder at the defect.