Machine Learning assisted interface analysis in MnAl-C

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The significance of permanent magnets in various technological applications, such as wind turbines, electric vehicle motors, and solar cell storage devices, cannot be overstated. As such, there is a compelling need for a deeper comprehension of their fundamental characteristics, including coercive fields, domain reversal phenomena, and hysteresis curves, in order to effectively engineer these features. Tremendous progress has been achieved in the field of computer simulations pertaining to these phenomena. While such simulations offer valuable insights into the aforementioned properties, they often entail significant computational efforts. Consequently, the predictive capabilities of machine learning models may offer a promising avenue to supplement these efforts and enhance our understanding further. In this study, we leverage a comprehensive database comprising results from numerous simulation runs across a variety of crystallographic twin scenarios in MnAlC magnets. MnAlC is a promising candidate for rare earth free permanent magnet twins where the twins interface heavily influence the coercivity.

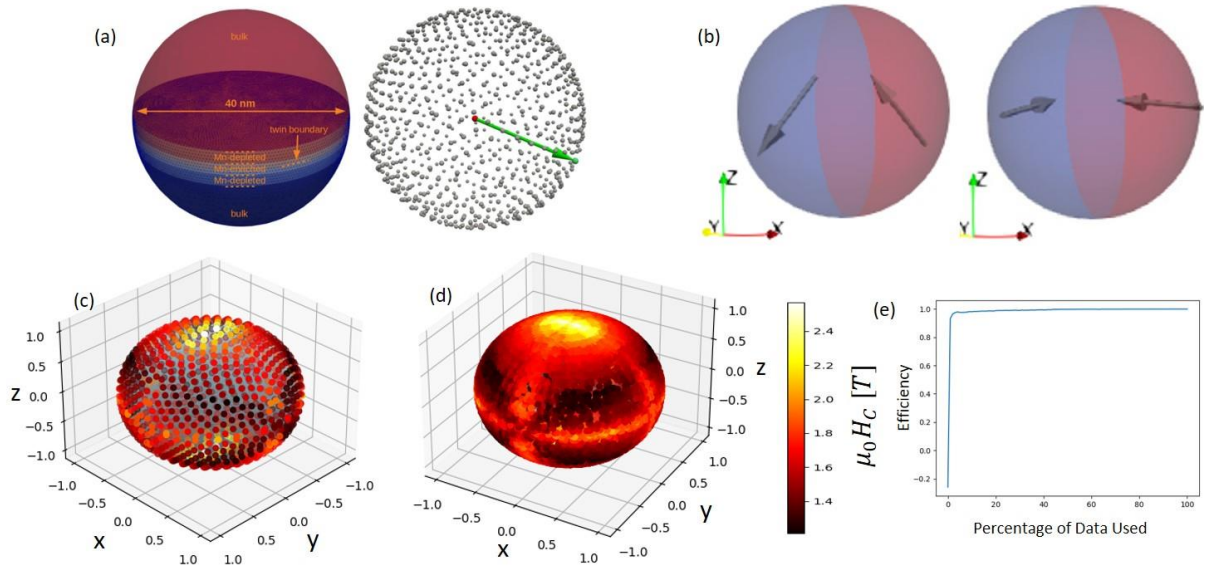

Figure 1. Finite element micromagnetic model of twin boundary and segregation layers (a left); external field directions evenly distributed around a unit sphere with the simulation model in the center (a right). Coherent twins (b left) and order twins (b right) with their respective easy axes (as arrows). Training (c) and predicted (d) coercive field values. Efficiency (1-Mse from xgboost metric) as a function of data used percentage (e).

In this study, we leverage a comprehensive database comprising results from numerous simulation runs across a variety of crystallographic twin scenarios [1]. The simulation models consist of a sphere, which is split by a twin interface, as shown in Fig. 1 (a) and (b) [1]. The misorientation angle between the magnetically easy axes of each entity was set to 75.66° and 95.35° for true and order twin boundaries, respectively. Demagnetization curves were computed by a fast micromagnetic solver [2], with external fields evenly distributed on the surface of a unit sphere pointing in the direction of its center, where the probe is located. Utilizing these results, the computed coercive field values of twin interfaces, as a

foundation, we employ ensemble methods such as random forests and gradient boosting, which typically shows good performance in micromagnetic systems [3], to predict coercive field for different external field orientations taking as features the angles which describe external field orientations. Remarkably, our testing phase demonstrates exceptionally high accuracy. Subsequently, we systematically reduce the volume of training data and compare the predictions with those derived from the full dataset. Our findings indicate that unless the dataset dimension is reduced to less than 10% of the original size, there is no significant deviation in the output (Fig. 1 on the right). This means, that it is possible to investigate only a few external field directions with respect to the twin boundary interface, to obtain a full description of the coercive field distribution of particular twin interfaces. This observation holds considerable significance, as it enables the redistribution of simulation efforts to explore new scenarios.

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