Challenges in magnetic materials modelling

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Abstract

Computational micromagnetics enables the design and development of magnetic materials and devices. However, accurately modelling magnetic materials presents several challenges. Often, input parameters and intrinsic material properties are unknown. This necessitates the use of ab initio simulations or estimations based on machine learning to determine these parameters. Microstructure significantly influences the hysteresis properties of magnetic materials. Generating synthetic microstructures that accurately represent real-world ones is a major challenge in magnetic material modelling. Another challenge arises from the discrepancy in length scales. Micromagnetic simulations demand a high-resolution computational grid to resolve features like domain walls, which are typically a few nanometres in size. In contrast, real magnets can be macroscopic, spanning several micrometres or larger. This scale difference necessitates efficient numerical methods and parallel computing to manage the computational demands. Reduced-order models offer an alternative approach, enabling simulations of larger magnets by simplifying the representation of the magnetic system [1]. One such method constructs the macroscopic demagnetization curve from local hysteresis models applied at representative points of the microstructure. This method relies on the calculation of the magnetostatic interaction field of uniformly magnetized grains, which can be efficiently performed using an integral approach accelerated by hierarchical matrices. We demonstrate this method for computing hysteresis properties of sintered permanent magnets.

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References

[1] Kovacs, A., Fischbacher, J., Oezelt, H., Kornell, A., Ali, Q., Gusenbauer, M., Yano, M., Sakuma, N., Kinoshita, A., Shoji, T., Kato, A. 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, 1094055 (2023).