Graph based coercivity prediction for core-shell type hard magnets

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Understanding the design of hard magnets is pivotal for using heavy rare earths efficiently. Among the hard magnets, the Nd-Fe-B sintered permanent magnets find various applications such as in health care, automotive industry and cooling devices [1]. When diffused with heavy rare-earths they form core-shell type main phase. This adds additional compositional and microstructural features on which the extrinsic property, like coercivity depends. Graphs can naturally represent complicated microstructures. Once trained, a graph neural network can predict the desired label of interest. However, due to GIGO principle a high quality training data is crucial for this purpose.

In this work we show our approach for generating the training data to predict coercivity by using machine learning and advanced micromagnetics. We sample the design variables to encompass the spread of simulation parameters for various microstructures. The intrinsic properties are predicted from composition of the magents with different diffusion profiles of terbium. We developed and applied a reduced order model [2] for micromagnetic simulations of the generated microstrucutres at realistic length scales. A graph neural network is then trained on simulated dataset using the architecture created by Moustafa *et al.* [3]. We predicted coercivity using this approach with R^2 score for training set ~ 0.93 and for test set ~ 0.81. Next, we coupled coercivity prediction with uncertatinity quantification. This work lays the basis for the inverse magnet design.

References:
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