Graph Neural Networks to Predict Coercivity of Hard Magnetic Microstructures

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ABSTRACT

Graph neural networks (GNN) are a promising tool to predict magnetic properties of large multi-grain structures, which can speed up the search for rare-earth free permanent magnets.
We use our Reduced Order Model (ROM) to generate a large training set of $Nd_2Fe_{14}B$ by the means of simulation. The simulated cubes differ in five parameters over a wide range as well in the individual grain shape and arrangement.
The dataset consists out of more than 700 of these cubic microstructures and is divided into training-, validation-, and testset with a ratio of 70/15/15.
The used GNN is built with the spektral library to incorporate convolutional layers with edge features. A dropout layer and the monitoring of validation and test loss during the training decrease the risk of overfitting which would result in a lower expressivness of the GNN. A final dense layer allows to have the coercivity of each graph as the label. We measure the performance of our trained GNN using the R^2-value of the test set. Training of the GNN was stopped using early stopping after ~2100 epochs, resulting in an R^2-value of 88 % for the test set. A satisfying accuracy. In further work, the generalisation ability of the GNN shall be investigated.

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1 Motivation

With the rapid progress of climate change, it is more urgent than ever to accelerate the green transition, especially in energy production e.g. offshore wind turbines and transportation e.g. electric vehicles. Consequently the demand for the rare-earth element neodymium, main component in NdFeB permanent magnets, will rise more than threefold until 2050 [1].
Since rare-earth elements are critical regarding price and supply stability, the content of rare-earth elements in such magnets need to be reduced while maintaining the performance. Micro- and nanostructural design was identified the most promising strategy to achieve this goal [2] [3]. To examine the effect of microstructural design changes on the magnets performance, simulations are a good means. To reduce the computational effort of simulations, in this work we focus on a graph neural network (GNN) layout to do an evaluation of the influence of different microstructural parameters on the magnet's performance. GNNs are found to be simple, accurate and having a good generalisation [4].

2 Graph Neural Network

A GNN is suitable because the microstructure can be abstracted to a graph, where the grain boundary phase is represented by edges, and respectively the grains by the nodes.

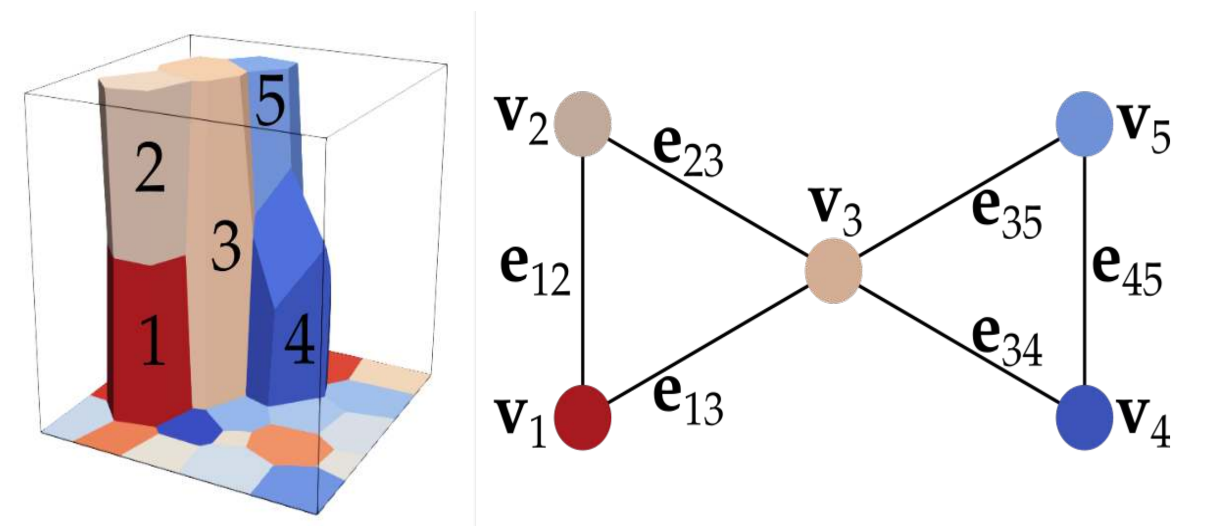

Fig. 1: Left: five selected grains of a cuboid grain structure. Right: The nodes correspond to the grains, including the grain features v_i. The edges e_{ij} correspond to the grain boundary phases between each neighbouring grain.

The used GNN, based on spektral, a GNN library built on Tensorflow, consists out of eight convolutional ECCConv layers with the each graphs' node and edge features, a global pooling layer, a dropout layer to prevent overfitting and make the model more robust, and finally dense layer for the graph regression task. The node features are different grain properties, the edge feature is the non magnetic grain boundary thickness and the graph label is coercivity.

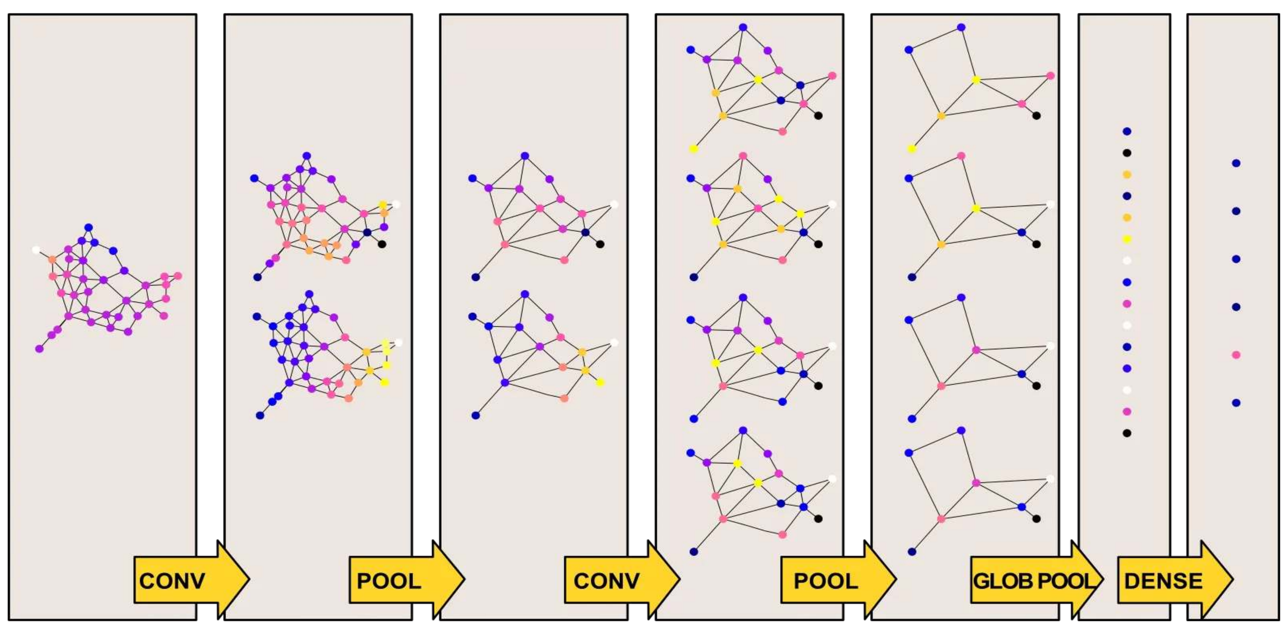

Fig. 2: Different layers and their function in a GNN [5].

3 Training

The dataset containing around 700 $Nd_2Fe_{14}B$ microstructures with a non-magnetic grain boundary phase was obtained with our Reduced Order Model (ROM) [6]. Using the ROM, a mean computation time for one sample of 6 min could be achieved. Fig. 3 shows the parameters and the respective range in which they were changed. A split into training/ validation/test dataset with the ratio 70/15/15 is done to ensure an expressive GNN. A manual hyperparameter tuning has been done. The model was trained for 2100 epochs, then the validation loss did not improve anymore and early stopping was applied to prevent overfitting.

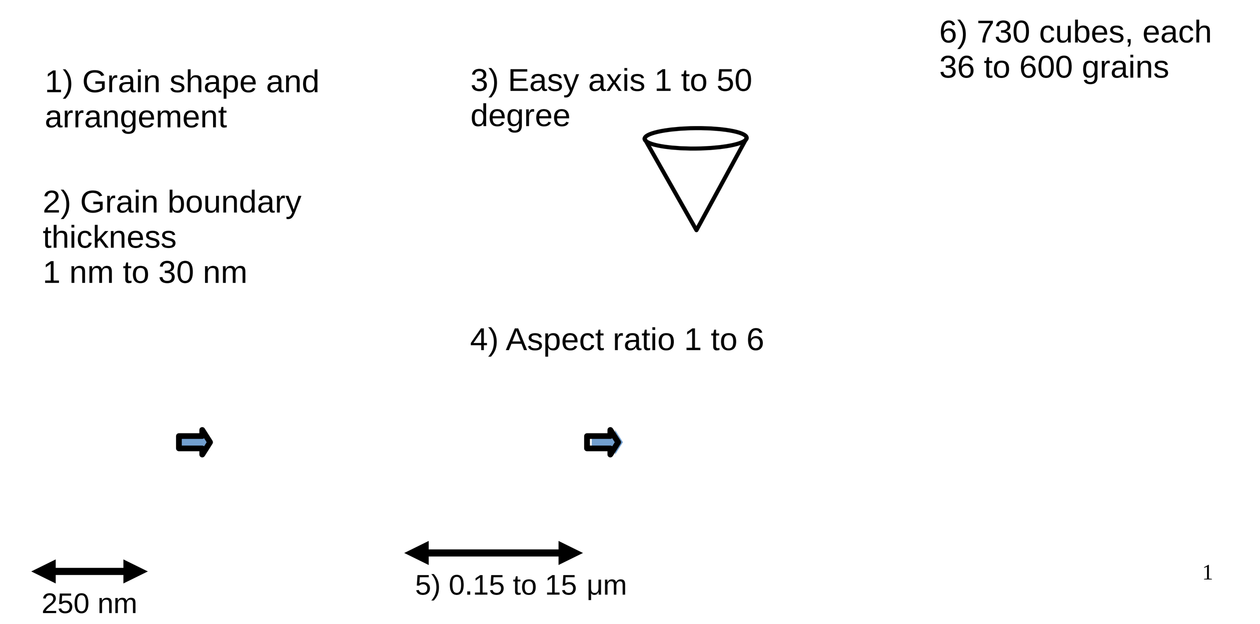

Fig. 3: 1) to 6) illustrates the different parameters and their respective range in which they were changed during dataset generation.

4 Results

The trained model has a satisfying accuracy. Most coercivity values are a bit higher predicted than computed, especially in the higher range. In a further step, the generalisation ability of the GNN shall be investigated.

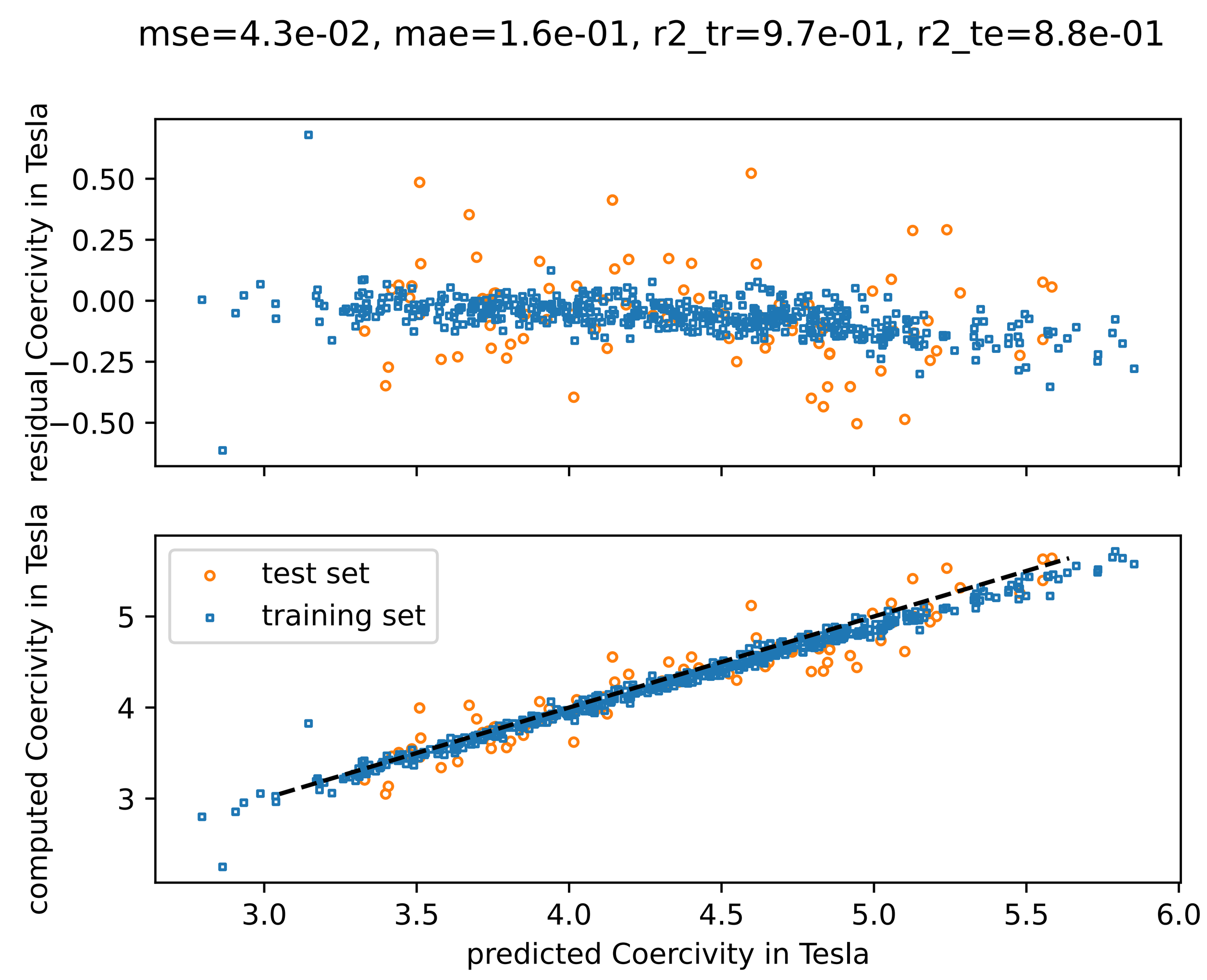

Fig. 4: Difference between prediction and computation of the coercivity, and the computed versus the predicted coercivity. The dashed lines represents zero-error for prediction. R^2 = 88% for the test set.

5 Conclusion

- GNN are a viable tool to predict coercivity of hard magnetic microstructures.
- In a next step, generalisation capabilities of GNN shall be investigated. Furthermore, inverse design could be used to enhance coercivity.

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