Combining micromagnetics and machine learning for the design of rare-earth lean permanent magnets

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The reduction of greenhouse gas emissions has become a global priority, with permanent magnets playing a key role in the electrification of transport and renewable energy systems. Growing demand of high-performance NdFeB-type magnets necessitate the development of alternatives with lower rare-earth content while maintaining the magnets' high coercivity and energy density product.
We follow two strategies on different length scales. At the nanoscale, our focus is on identifying optimal spatial compositions of magnetically hard and soft phases, aiming to maximise the energy density product BH_{max} while reducing the reliance on rare-earth-containing hard phases.[1] On the microscale, we target enhancements in coercivity through tailoring of microstructure and chemical composition. Machine learning serves as a vital tool in advancing both approaches.
To evaluate BH_{max} of different spatial phase distributions, we segment a cube into smaller patches of either magnetically hard $Nd_2Fe_{14}B$ or soft $Fe_{65}Co_{35}$ material, and micromagnetically compute their demagnetization curves. An optimization framework, incorporating an adapted binary search algorithm [2], was developed to propose new promising design canditates. To speed up the optimizer, a convolutional neural network is used as a surrogate model. The network was trained on the micromagnetic results to predict BH_{max} from the spatial arrangement of the patches.
To investigate microstructure on the microscale, a reduced order model for hard magnetic materials [3] was developed, significantly extending the length scale limits of micromagnetic computations. Using this model, we calculate the coercive field of magnetic cubes with edge lengths of up to 70µm and varying microstructures. We exploit the fact that granular structures can be well described as graphs and train a graph neural network on the simulation results to predict the coercive field based on various microstructural properties. This model can be used to find beneficial microstructural properties by inverse design.

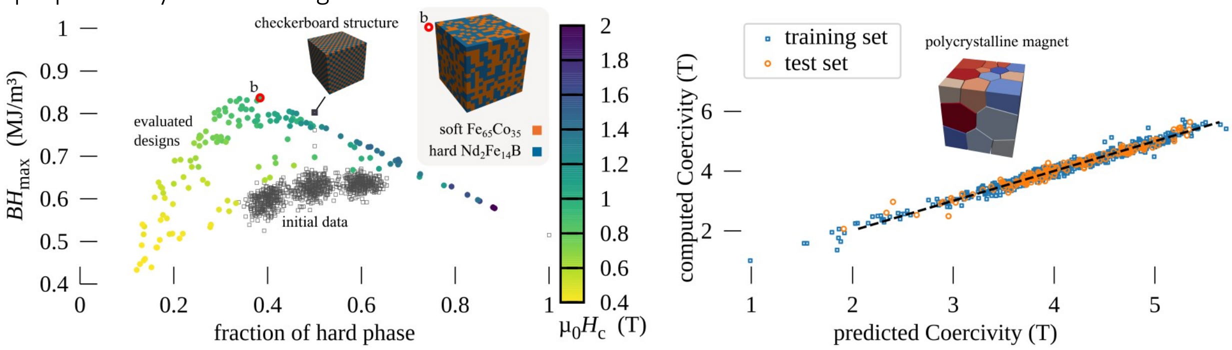

Figure 1. *Left*: Hard/soft magnetic spatial distributions proposed by a trained convolutional neural network model and evaluated by micromagnetic simulations. The design with the highest energy density product so far (b) is shown in the corner. *Right*: Computed versus predicted coercive field of a granular magnetic cubes of various sizes and microstructure. A graph neural network was tuned to achieve a high prediction accuracy with R^2=96%.

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References

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