

# MS09 MACHINE LEARNING AND COMPUTATIONAL MICROMAGNETISM: CLASSIFICATION AND OPTIMIZATION OF A MAGNET'S MICROSTRUCTURE

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## ABSTRACT

We present an automated search and optimization tool for the granular microstructure of permanent magnets. Machine learning is a method to relate microstructure and hysteresis properties of a permanent magnet. Once built, the model can be used to replace time consuming micromagnetic simulations as design tool that predicts coercivity quickly. The machine learning tool chain needs (i) features characterizing a magnet's microstructure, (ii) fast methods for data generation, (iii) a machine learning predictor trained to predict hysteresis properties for a given microstructure, and (iv) a model of validation and interpretation. We developed an automated tool for the optimization and design of the core-shell structure in a permanent magnet. A deep Bayesian optimizer [1] is used to sample a high dimensional feature space for the grain. A finite element model reflecting a specific feature set is generated and coercive field is computed. Evaluating different machine learning models for predicting coercivity, we achieved the best regression scores with a gradient boost model.

## REFERENCES

- [1] F. Häse, L. M. Roch, C. Kreisbeck, A. Aspuru-Guzik. *Phoenix: A Bayesian Optimizer for Chemistry*, ACS central science 4.6 (2018): 1134–1145.

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