

The coercivity of permanent magnets: Insights from micromagnetics and machine learning

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Permanent magnets are of utmost importance for the transition to a carbon free economy. Permanent magnets are essential for effective power generation and transformation. A key property of a permanent magnet is its coercive field. Micromagnetic simulations and machine learning help to understand the coercivity mechanism of permanent magnets, which in turn can guide the optimization of magnetic materials for specific applications.

Magnetization reversal starts locally. Simulations of the demagnetization process of (NdLaCe)FeB-based magnets show that the sum of the external field and the demagnetizing field evaluated at a distance of 1.44 times the exchange length determines the switching field of a grain [1]. This finding expresses the balance of exchange and magnetostatic interactions which in turn leads to a decrease of the coercive field with increasing grain size. Furthermore, magnetostatic interactions cause a cascade type magnetization reversal in large-grained magnets. Once a grain is reversed, its magnetostatic field triggers the reversal of its neighbours. Simulations of the coercive field of magnets with an ideal microstructure, in which the grains are separated by a non-magnetic grain boundary phase, show that demagnetizing fields and misalignment cause a drastic reduction of the coercive field. For uniformly distributed anisotropy directions with a maximum misorientation of 35 degrees, the computed coercive field is 3.4 T, 2.8 T, 2.3 T, 1.8 T, and 1.3 T for an average grain size of 0.1 μm , 0.5 μm , 1.8 μm , 7.3 μm , and 29.3 μm , respectively.

Micromagnetic simulations show, that already a thin anisotropy defect reduces the switching field compared to its value expected from the Stoner-Wohlfarth theory. Deviations from the angle dependence of the switching field from the Stoner-Wohlfarth curve indicate the presence of defects.

Machine learning combines available data sets into coercivity models. Model interpretation helps to identify trends and show how key material properties such as the chemical composition, grain size, and defect thickness, influence the coercive field.

References:

[1] A. Kovacs et al., *Front. Mater.* **9**, 1094055 (2023)

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