Micromagnetic optimization of permanent magnetic materials

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The development of permanent magnets containing less or no rare-earth elements is linked to profound knowledge of the coercivity mechanism. Prerequisites for a promising permanent magnet material are a high spontaneous magnetization and a sufficiently high magnetic anisotropy. In addition to the intrinsic magnetic properties the microstructure of the magnet plays a significant role in establishing coercivity. The influence of the microstructure on coercivity, remanence, and energy density product can be understood by using micromagnetic simulations. With advances in computer hardware and numerical methods, hysteresis curves of magnets can be computed quickly so that the simulations can readily provide guidance for the development of permanent magnets. In particular micromagnetic simulation can address the impact of grain size and grain shape on coercivity. The simulations show that for rare-earth free phases such as $L1_0$ FeNi small, needle shaped grains are beneficial. A small grain size becomes increasingly important if the chemical ordering of L10 FeNi is imperfect. Similarly, elongated grains can improve coercivity in $Nd_2Fe_{14}B$ magnets provided that the grain boundary phase is paramagnetic. Grain boundary phases are shown to impact coercivity considerably. Grain boundaries and interfaces may act both as pinning and as nucleation site. If two grains are in direct contact and exchange coupled, partial domain walls form at the interface between the grains. From there reversed domains can easily nucleate. This effect reduces the coercive field in rare-earth reduced permanent magnets in the $ThMn_{12}$ structure to about 10 percent of the anisotropy field. By computing the energy barrier for thermally induced magnetization reversal, micromagnetic simulations can show the weak spots in the microstructure, where magnetization reversal is initiated.

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