Magnetic anisotropy in iron-based rare-earth compounds

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Abstract:

Modern high-performance permanent magnets mainly consist of 3d transition-metals and rare-earth elements. High saturation magnetization and high Curie temperature originate predominantly from interacting 3d electrons, whereas the 4f electrons play a crucial role in strong magnetocrystalline anisotropy (MCA). There is no established way of accurately calculating MCA of rare-earth magnets from first-principles, mainly because localized 4f electrons are difficult to treat [1]. A conventional scheme is based on crystal-field theory. We present first-principles evaluation of crystal-field parameters, and discuss how chemical doping affects MCA through change in electronic states [2,3]. We also discuss finite-temperature MCA using a classical spin model and constrained Monte Carlo method [4].

References:

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