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Hysteretic properties of Nd2Fe14B-based permanent magnets: First principles and micromagnetic modeling ALEKSANDER WYSOCKI, DENIS KUKUSTA, LIQIN KE, VLADIMIR ANTROPOV, Ames Laboratory, Ames IA 50011 — We combine ab initio electronic structure calculations with micromagnetic simulations to investigate permanent magnet properties of Nd2Fe14B-based systems. First, magnetic moments, anisotropy constants and exchange interactions of bulk Nd2Fe14B are calculated from first principles. These parameters are then used to construct a micromagnetic model for realistic samples and evaluate hysteresis loop at finite temperatures using Monte Carlo method. Several generic microstructures are considered including randomly oriented grains, hard/soft multilayers, and core/shell geometries. We find optimal grain sizes and hard phase/soft phase volume ratio which maximize maximum energy products of the systems. Further, we discuss the nature of the thermal spin reorientation effect in the bulk material and how it affects the finite temperature hysteretic properties.

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