Theoretical limit of Maximum Energy Product of Rare-earth Free Core-Shell Nanomagnets

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Theoretical calculation of maximum energy product, $(BH)_{max}$, of core-shell nanomagnet, that a magnet designer needs, is lacking. Therefore, first-principles calculations were performed for ordered MnBi [1], MnBi-Co(Fe) [2], τ -MnAl [3], and strontium ferrite (SrFe₁₂O₁₉) [4,5], to calculate the saturation magnetization (M_s), effective anisotropy constant (K_{eff}), and Curie temperature (T_c). These materials are magnetically hard, thereby core material candidates. Linear-augmented plane wave (FLAPW) and linear-muffin-tin-orbital (LMTO) calculations based on density functional theory (DFT) within the local spin density approximation (LSDA) are used to obtain magnetic properties of the core materials.

With regards to calculation of $(BH)_{max}$ of core-shell nanomagnet, we have used both Hong-Bae's analytical model [6], which is based on the magnetic anisotropy constant (*K*), and Hong-Park's model based on the intrinsic coercivity (H_{ci}) [7].

It was found that the $(BH)_{max}$ of core-shell was increased by 129% for core MnAl, 308% for MnBi, and 206% for SrFe₁₂O₁₉. Nano-maufacturing of core-shell nanomagnets is challenging.

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