Theoretical Study of Rare-Earth Lean Magnet Compound $NdFe_{12}N$

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The $ThMn_{12}$-type iron-based rare-earth compounds have attracted interest as potential strong permanent magnet compounds because of their high iron content (low rare-earth content) which is favorable for achieving large magnetization. Recently, $NdFe_{12}N$ film has been synthesized [1] following first-principles calculation [2], and it was reported that $NdFe_{12}N$ exhibits larger saturation magnetization and anisotropy field than those of $Nd_2Fe_{14}B$. Here we present a theoretical study of this compound. Our first-principles calculations show that magnetism in $NdFe_{11}TiX$ and $NdFe_{12}X$ for X=B,C,N,O,F is sensitive to X. The magnetization is substantially larger for X=N,O,F than for X=B,C, while the magnetocrystalline anisotropy becomes the strongest for X=N [3]. Analysis using a classical spin-model clarifies that the magnetic anisotropy above the room temperature is strongly influenced by the exchange coupling between Fe and Nd [4,5]. We also report the effect of the third element M (M=Ti,V,Cr,Mn,Co,Ni,Cu,Zn) on the energetics and magnetism in $NdFe_{11}M$ [6].

References

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