First Principles Study on Effects of Substitutionally and Interstitially Doped Elements in NdFe\textsubscript{11}MA

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The $RT_{12-x}M_x$ compounds and their nitrides, having the ThMn\textsubscript{12} structure, are candidates for high-performance permanent magnets, since they have large iron content and thus large magnetization. Although $RFe_{12}$ is thermodynamically unstable, substitution of a part of iron atoms by other elements, e.g. titanium, stabilizes the compound. It is known that interstitial nitrogenation of the neodymium 1-12 type materials exhibits strong uniaxial anisotropy [1]. However, effects of substitution and interstitially doped elements on magnetic properties are still to be understood from microscopic viewpoint.

We study magnetic properties of NdFe\textsubscript{11}MA ($M$ is, ex. 3d transition metal and $A$ is N, B, C, O and F) that are related to strong ferromagnets containing rare-earth elements. The crystal electric field parameter $A_{20}$ at the Nd site is calculated using the density functional theory in the generalized gradient approximation and the open-core treatment for the Nd-f states. We found that substitution of the iron atom at the 8$i$ site with titanium is preferable as observed in the experiments. Titanium substitution affects both magnetization and magnetocrystalline anisotropy. The magnetization is substantially suppressed by the substitution. The system substituted at the 8$i$ site shows positive value for $A_{20}$ i.e. uniaxial anisotropy while a calculation of NdFe\textsubscript{12} gives negative $A_{20}$. We found that the anisotropy depends on distribution of titanium atoms. Interstitial nitrogenation also affects the magnetic properties. The magnetization is increased and the uniaxial anisotropy is enhanced by interstitial nitrogenation as observed in the experiments. We apply the analysis to other elements. Detailed analysis on the substitutional and interstitially doped element dependence will be presented.

References:

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