First principles study on effect of stabilizing element M in $NdFe_{11}M$

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Recent experiment succeeded epitaxial growth of a film sample of $NdFe_{12}N$. The sample shows larger magnetization and stronger magnetocrystalline anisotropy than $Nd_2Fe_{14}B$ [1]. $NdFe_{12}N$ and its related materials can be expected as good candidates for the permanent magnet materials [1,2]. $NdFe_{12}N$ is synthesized from $NdFe_{12}$ by interstitial nitrogenation to enhance the magnetization and the magnetocrystalline anisotropy (see Ref [3] for the effect of nitrogenation). Even though the epitaxial growth of $NdFe_{12}$ is succeeded, synthesis of the bulk sample is still difficult. To stabilize the materials, third elements, ex.) Ti, have been used, but the magnetization is reduced by the substitution [4]. For the stabilizing elements, much stability with less amount of substitution and less reduction of the magnetization are required.
The purpose of this study is to find better stabilizing elements for $NdFe_{11}M$ in terms of the stability, the magnetization, and the magnetocrystalline anisotropy. We perform the first principles calculation of $NdFe_{11}M$ (M=Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn) and estimate the stability, the magnetization, and the magnetocrystalline anisotropy.
The calculation is performed by using QMAS [5] based on the density functional theory and the projector augmented-wave method. The exchange-correlation energy functional is approximated by using the generalized gradient approximation. Nd-4f electrons are treated as open-core states. The magnetocrystalline anisotropy is estimated from the crystal field parameter A_2^0.
To estimate the stability of $NdFe_{11}M$, we calculate the formation energy by M substituted with Fe. The formation energies for Ti, V, Cr, Mn give negative values, and especially Ti stabilizes the alloy more than other elements. In experiments, these alloys are indeed observed and the amount of substitution of Ti is less than other elements. We found that Co, Ni, Zn also give negative formation energies, and that the stability of $NdFe_{11}Co$ are comparable to that of $NdFe_{11}Ti$. $NdFe_{11}Co$ has as large magnetization as $NdFe_{12}$. Nitrogenation enhances the magnetization of $NdFe_{11}Co$. For the magnetocrystalline anisotropy, nitrogenation enhances the crystal field parameter as well as $NdFe_{12}$ and $NdFe_{11}Ti$. This indicates that the uniaxial anisotropy is enhanced by nitrogenation.
As conclusion, Co is a good stabilizing element for $NdFe_{11}M$.
In our talk, we will also discuss the effect of Zr substitution.

Reference
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