Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

First principles study of doping effects in $NdFe_{11}Ti$ permanent magnet compound YOSUKE HARASHIMA, NRI, "RICS," AIST; ESICMM, NIMS, KIYOYUKI TERAKURA, NRI, "RICS," AIST; NIMS, HIORI KINO, MANA, NIMS; ESICMM, SHOJI ISHIBASHI, NRI, "RICS," Green-Innovative Magnetic Material Research Center, AIST , TAKASHI MIYAKE, NRI, "RICS," ESICMM, NIMS, Green-Innovative Magnetic Material Research Center, AIST — Permanent magnet compounds are required to have large magnetization and strong uniaxial magnetocrystalline anisotropy. $NdFe_{11}Ti$ which is one of the $ThMn_{12}$-type rare-earth 3d-transition metal compounds has large magnetic moment due to its high content of Fe. The magnetization and magnetocrystalline anisotropy of the compound can be tuned by nitrogen doping at interstitial sites. $NdFe_{11}TiN$ is a good candidate for a permanent magnet compound. Then, it is interesting whether there is another dopant that enhances the magnetic properties. We have investigated doping effects of $NdFe_{11}TiX$ where X=B, C, N, O, and F by using first principles calculation. These dopants increase the magnetization, and the increase is especially large for N, O, and F doping. The magnetocrystalline anisotropy is estimated from the crystalline electric field parameter $<r^2>A_2^0$. $NdFe_{11}TiB$ has negative value of $<r^2>A_2^0$ that implies the compound has in-plane anisotropy. As the atomic number of the dopant increases from B to N, $<r^2>A_2^0$ is increased, and $NdFe_{11}TiN$ has a large positive value, suggesting strong uniaxial anisotropy. Then, $<r^2>A_2^0$ turns to decrease as the dopant is changed from N to O to F, and $NdFe_{11}TiF$ has a large negative value. In conclusion, we found that N is the most appropriate dopant among B, C, N, O, and F.

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Date submitted: 14 Nov 2014 Electronic form version 1.4