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First-Principles Calculations of Magnetocrystalline Anisotropy in NdFeB Type Magnet Materials

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NdFeB sintered magnet is used in a variety applications because of its excellent magnetic feature. But there is a commercial resource procurement risk, because almost of Nd metal is produced in China. It is reported that the magnetic anisotropy of Nd on 4f site in $Nd_2Fe_{14}B$ is smaller than that on 4g site [1]. Therefore, if the Nd on 4f site is selectively replaced another Rare-Earth (RE) elements, it may be possible to develop the NdFeB type sintered magnet which contains less Nd, without lowering the magnetic properties. In this study, the site preference of RE in $NdREFe_{14}B$ are revealed by first-principles calculations. In addition, quantitative investigation of magnetocrystalline anisotropy of $NdREFe_{14}B$ are performed.

In this study, all of the first-principles calculations were performed by the projector-augmented wave (PAW) method within generated grained approximation Perdew-Burke-Ernzerhof revised for solids (GGA-PBEsol) implemented in VASP code [2,3]. The cutoff energy was set to 400eV. Numerical integration was carried out at $6\times6\times3$ points in a Brillouin zone. The on-site Coulomb term (U=6eV) were applied for 4f electrons of RE [4]. The site preference of RE in NdREFe14B was evaluated by calculating the difference of total energy between RE on 4f site and on 4g site. The magnetocrystalline anisotropy was calculated by traditional point charge model and the valence of each element was evaluated by Bader Charge Analysis [5].

Fig.1 shows the site preference of RE in $NdREFe_{14}B$. The horizontal axis is RE and the vertical axis the deference of total energy between 4f site substitution and 4g site substitution. Y and Ce prefer 4f site substitution. On the other hand, La prefers 4g site substitution. However, the difference of total energy is relatively small (< 1eV). It may mean that Y, La and Ce occupy not only 4f site but also 4g site.

Fig.2 (a) shows the calculated anisotropy constant K_1 of $Nd_2Fe_{14}B$. The blue area means the partial K_1 of Nd which is on 4f site, and red area means that of on 4g site. The sum of blue it and red it means the entire K_1 of $Nd_2Fe_{14}B$. The partial K_1 of Nd which is on 4f site is smaller than that of on 4g site. These calculated results are qualitatively agreed with the experimental results [1]. Fig.2 (b) shows the entire calculated anisotropy constant K_1. The horizontal axis is RE in $NdREFe_{14}B$, the vertical axis is calculated K_1. The blue bar is the calculated K_1 when RE is on 4f site in $NdREFe_{14}B$, and red bar is the calculated entire K_1 when RE is on 4g site. When RE is Sm, Er and these are on 4g site, the K_1 shows negative value because the sign of Stevens factor of Sm, Er is different from that of Nd. On the other hand, if it is considered that RE occupies randomly 4f and 4g site, the calculated K_1 of $NdREFe_{14}B$ is given the average of both blue bar and red bar. The calculated K_1 of $NdYFe_{14}B$, which Y replaces the half on Nd in $Nd_2Fe_{14}B$ is about 75% of that of $Nd_2Fe_{14}B$. And the K_1 of $NdHoFe_{14}B$, which Ho replaces the half on Nd in $Nd_2Fe_{14}B$ is as same as that of

$Nd_2Fe_{14}B$. Therefore, there is a possibility of obtaining more than half of the magnet material properties of $Nd_2Fe_{14}B$, even if the half of Nd in $Nd_2Fe_{14}B$ is replaced another RE.

References

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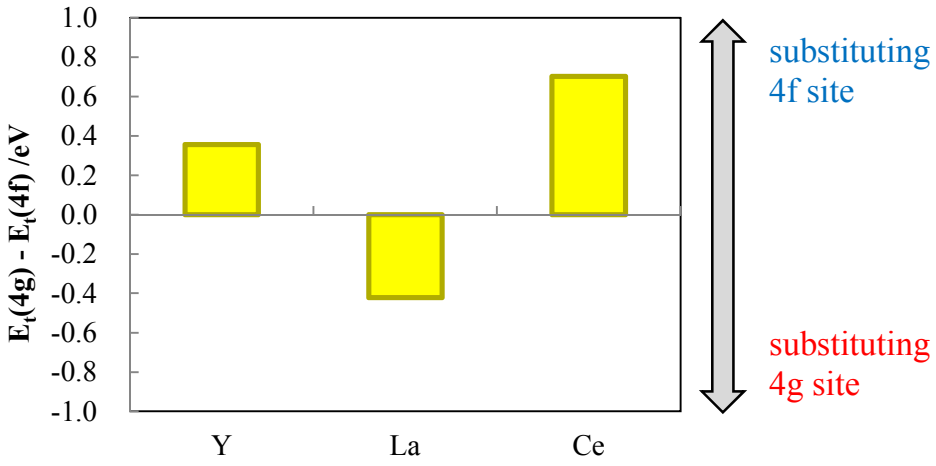

FIG.1 Calculated site preference of $NdREFe_{14}B$ (RE=Y, La, Ce)

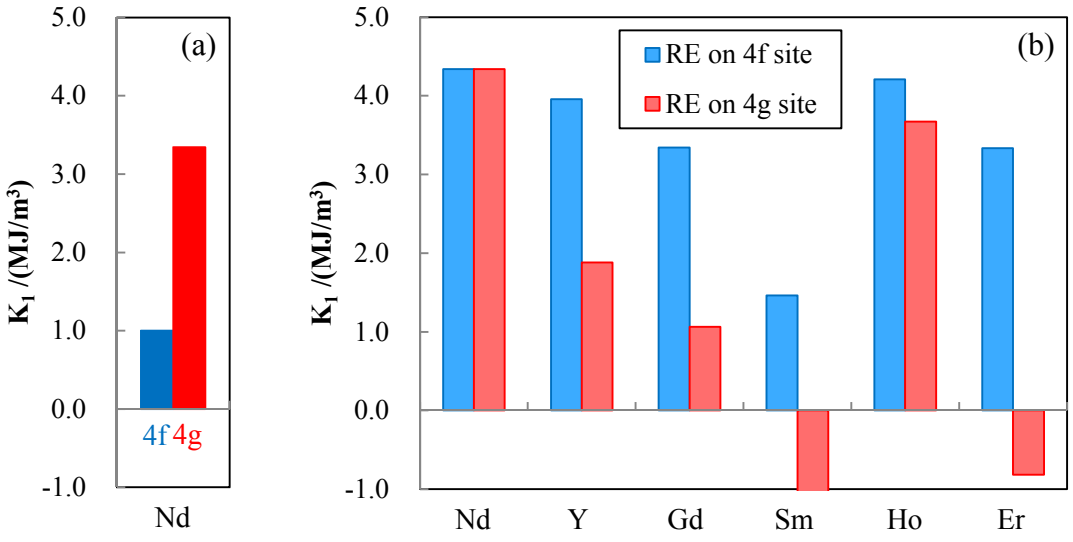

FIG.2 (a) Calculated partial anisotropy constant K_1 of Nd2Fe14B
(b) Calculated anisotropy constant K_1 of $NdREFe_{14}B$ (RE=Nd, Y, Gd, Sm, Ho, Er)