Analysis of magnetic properties for 1-12 rare-earth intermetallics based on first-principles

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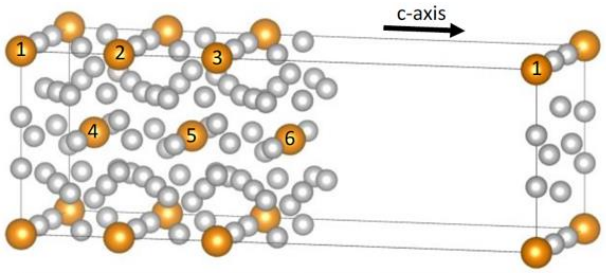
Due to increasing demands for high performance hard magnets for applications like wind turbines or electric vehicles, intensive studies have been carried out to investigate novel magnetic materials with comparable magnetic properties to $Nd_2Fe_{14}B$. Among them, because of high fraction of iron, rare-earth iron intermetallic compounds in ThMn12 structure have attracted constant attention. In particular, the nitrogenated compounds $NdFe_{12}N$ and $NdFe_{11}TiN$ stimulated much more interest among this series of compounds both experimentally and theoretically [1, 2]. The other 1-12 type intermetallics studied by screening approach, where the magnetic properties such as anisotropy fields and maximum energy products are estimated in a systematic way [3].

Motivated by these background, here we focus on *R*Fe12 with *R*=Nd or Sm and investigate their magnetic properties theoretically. First, we calculate the basic magnetic properties such as magnetic moment and magnetic anisotropy of each ion, and then define a crystal field Hamiltonian for *R* ions based on first-principles calculations to construct an effective spin model for these systems. We also carry out the electronic state calculation for these systems with simple surfaces. This is because, we have found that the Nd ions exposed on the (001) surface of the $Nd_2Fe_{14}B$ structure not only lose their uniaxial anisotropy but also exhibit in-plane anisotropy. Here we call such Nd ions as anomalous Nd, and we can expect that the same thing happens also *R*Fe12 systems. Then we carry out spin-dynamics calculations for the effective spin model including the information of surface *R* ions to estimate the expected values of coercivity.

Fig. 1 shows the (001) surface model structure, or the so-called slab model structure, for $NdFe_{12}$ system, as an example. The leading crystal field parameter A20's are shown in the figure. The 1st and 6th Nd ions show the strong c-plane anisotropies. Thus we find that the Nd on the surfaces can be anomalous even for the NdFe12 system. We will also discuss the effects of anormalous *R* (*R*=Nd, Sm) ions for the coercivity in the 1-12 type rare-earth intermetallic compounds.



Nd	1	2	3	4	5	6
$A_2^0\langle r^2\rangle$ (K)	-488.4	45.8	-20.9	-8.7	-16.7	-397.0

Fig. 1 Cristal field parameters in NdFe12 surface model

[1] T. Miyake, K. Terakura, Y. Harashima, H. Kino, and S. Ishibashi, J. Phys. Soc. Jpn. **83** (2014) 043702.

[2] Y. Hirayama, Y. K. Takahashi, S. Hirosawa, K. Hono, Scr. Mater. **95** (2015) 70.
[3] W. Körner, G. Krugel, and C. Elsässer, Sci. Rep. 6 (2016) 24686.