Powder neutron diffraction study for magnetism of rare-earth in $(Nd,Ce,La)_2Fe_{14}B$

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Introduction

To reduce expensive Neodymium in rare-earth magnets $Nd_2Fe_{14}B$ without decrease of magnetic properties, cheap Cerium is paid attention. In general, the Ce atom is in non-magnetic Ce^{4+} state. However, when the magnetic Ce^{3+} state is stable, the Ce should work as a substitution for Nd. Previous research reported that the larger ionic radii rare-earth prefer the larger cell volume [1]. The magnetic Ce^{3+} state has larger atomic radii (1.15 Å) than that of Ce^{4+} state (1.01 Å) [2]. Therefore, the La (1.17 Å) is doped as a spacer to stabilize the Ce^{3+} state. Previous powder neutron diffraction study reported that Ce atom in $(La,Ce)_2Fe_{14}B$ has no moment [3]. Following the previous results, in this study, powder neutron diffraction experiments were performed on $(Nd,Ce,La)_2Fe_{14}B$ to evaluate the rare-earth moment and the Ce state.

Experimental

The powder samples of $Nd_2Fe_{14}B$, $(Nd_{0.75}Ce_{0.225}La_{0.075})_2Fe_{14}B$, $(Nd_{0.5}Ce_{0.375}La_{0.125})_2Fe_{14}B$, and $Ce_2Fe_{14}B$ were measured. The mass of samples is 5g each. Diffraction patterns were gathered on the Echidna – High-Resolution Powder Diffractometer in Australia's Nuclear Science and Technology Organization (ANSTO). Natural boron was substituted with ^{11}B due to strong neutron absorption. The wavelength of the neutron is 2.44 Å.

Results

Figure 1 shows an observed diffraction pattern of $(Nd_{0.5}Ce_{0.375}La_{0.125})_2Fe_{14}B$ together with a result of Rietveld analysis. The experimental data was well explained by the calculated pattern. Figure 2 shows the obtained Nd content dependences of rare-earth moments. The moment sizes change linearly at Nd 70 % compounds. In contrast, at Nd 50 %, the moment size of 4*g* site deviates from linear change and increases. The reported rare-earth moments in $(Nd,Ce)_2Fe_{14}B$, shown as open triangles in Fig. 2, quickly decreases with decreasing Nd content [3]. This result suggests that some Ce atoms in 4*g* site are magnetic Ce^{3+} state instead of non-magnetic Ce^{4+} state thanks to the La atom spacer. The details will be discussed.

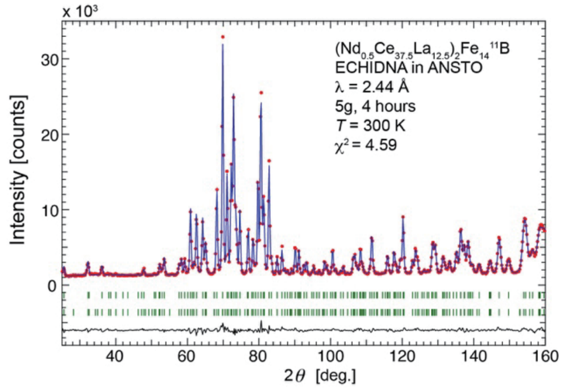

Fig. 1: The diffraction pattern of $(Nd_{0.5}Ce_{0.375}La_{0.125})_2Fe_{14}B$ together with Rietveld refinement results at 300 K.

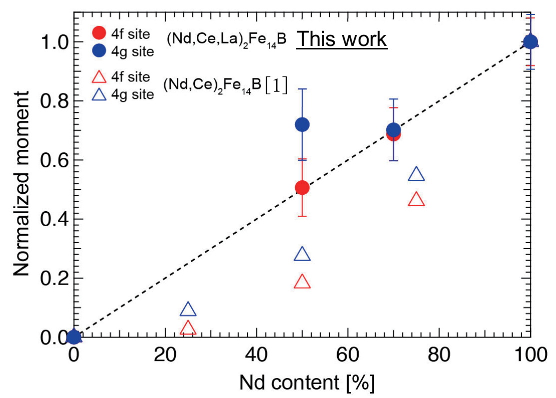

Fig. 2: The Nd content dependence of rare-earth moments at 4*f* and 4*g* site. The Moments shows here are normalized by the Nd moments of $Nd_2Fe_{14}B$.

Reference

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2) R. D. Shannon, Acta Crystallographica **A32**, 751 (1976).
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