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Site occupancy of Zr in the HDDR processed and melt-quenched $Nd_{12.5}Fe_{bal}Zr_{0.5}B_{6.2}$ magnets

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Introduction

HDDR process and rapid solidification process (melt-quench) for the $Nd_2Fe_{14}B$ with a small Zr additive contribute to improve of the coercivity and the remanence [1-4]. However, the role of Zr in the processes is not well understood. In order to know the role of small Zr additive in the HDDR process and the rapid solidification process for $Nd_{12.5}Fe_{bal}Zr_{0.5}B_{6.2}$, we carried out XAFS measurements of the Zr K edge.

Experiment

An ingot of $Nd_{12.5}Fe_{bal}Zr_{0.5}B_{6.2}$ alloys was prepared by arc melting under Ar gas atmosphere, subsequently homogenized in Ar gas at 1000°C for 40h. Disproportionation is carried out under the hydrogen pressure of 0.1MPa at 780°C for the homogenized sample. Recombination is done at 780°C under the hydrogen pressure of $<10^{-2}$Pa for 30min. Melt-quenched ribbon samples were prepared from the arc-melted ingot using a single-roller melt-spinning apparatus. The surface velocity of a Cu roll was 7.5m/s. Results of the X-ray diffraction using Cu Ka radiation for the ribbon samples show $Nd_2Fe_{14}B$ structure with the preferred orientation of c-plane for perpendicular direction to the roll surface.

XAFS measurements of the Zr K-edge for the homogenized state, the disproportionated state, the recombined state in HDDR process and for the melt-quenched sample were carried out at the temperature 20 K at BL9A by fluorescence method. Incident energy was selected by a double Si(111) crystal monochromater.

Results and Analysis

After the usual background subtraction and normalization, $\chi(k)$ was deduced using program AUTOBK. Figs. 1 and 2 show the observed $\chi(k)$ curves (solid line) for the Zr K-edge of the $Nd_{12.5}Fe_{bal}Zr_{0.5}B_{6.2}$ for the three states in HDDR process and for the melt-quenched sample respectively. Fitting calculations to these observed XAFS curves were done using FEFFIT program. The best fitting was obtained by putting Zr at ZrB_2 for the HDDR process (Fig. 1). While, the melt-quenched sample shows the best fitting for Zr to sit at Nd(4f) site in $Nd_2Fe_{14}B$ structure (Fig. 2).

Good agreement of the observed and the calculated curves mean that site occupancy of Zr is different by the sample preparation condition. It is thought that stable ZrB_2 compound has been already formed during arc melting, so that disparity of magnetic properties between the arc melting and the melt-quench seems to be attributed to the site different occupancy of Zr.

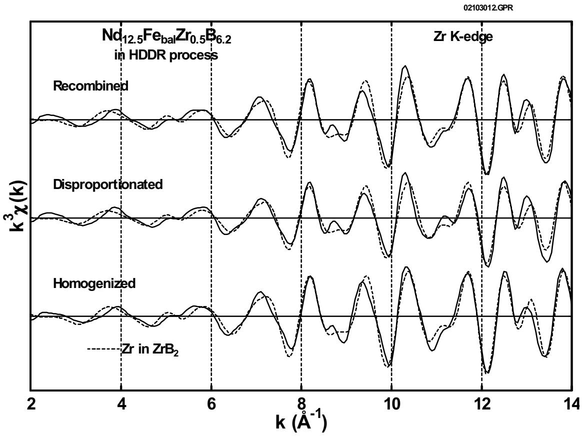

Fig. 1. XAFS spectra of the Zr K-edge of $Nd_{12.5}Fe_{bal}Zr_{0.5}B_{6.2}$ for the homogenized state, the disproportionated state and the recombined state. The solid lines are the observed results, and the broken lines the calculated ones for Zr in ZrB_2.

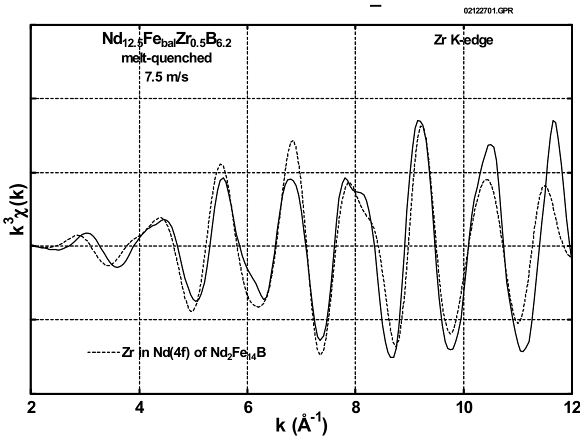

Fig. 2. XAFS spectra of the Zr K-edge of $Nd_{12.5}Fe_{bal}Zr_{0.5}B_{6.2}$ for the melt-quenched sample. The solid lines are the observed results, and the broken lines the calculated ones for Zr in Nd(4f) site of $Nd_2Fe_{14}B$.

References

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