Local structure of transition metal doped α"-Fe$_{16}$N$_2$

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1 Introduction

α"-Fe$_{16}$N$_2$ has attracted much attention because of its higher magnetization than α-Fe. Recently, our group reported that the highest magnetization value of 210 Am^{2}kg^{-1} was observed in a mixture of α"-Fe$_{16}$N$_2$ and α-Fe at 60wt% of the α"-Fe$_{16}$N$_2$ [1]. Their magnetic coercivity was above 50mT and increased with the α"-Fe$_{16}$N$_2$ content. Magnetic coercivity of the iron nitride should be managed to utilize the large magnetization as in either soft or hard magnet.

Cobalt doping into iron compounds has been reported to change their magnetic coercivity. Fe-Co bcc alloy shows the lowest magnetic coercivity of 1.5mT at 8at% of Co doping, which is about half of the value of the pure Fe [2]. On the other hand, Co doping into γ-Fe$_2$O$_3$ increased its magnetic coercivity above 60mT [3].

In this study, preparation of bulk powder product of Co doped α"-Fe$_{16}$N$_2$ through low temperature nitridation of fine powder of Fe-Co alloys obtained by hydrogen reduction of (Fe,Co)$_3$O$_4$ oxides and the local structure around the Fe and Co atoms in the nitride products were investigated.

2 Experiment

(Fe$_{1-x}$Co$_x$)$_3$O$_4$ fine powders obtained from Fe(acac)$_3$ and Co(acac)$_3$ in benzyl alcohol were reduced at 400 °C for 10 h in H$_2$ flow of 50ml/min. The reduced products were nitrided at 150 °C for 5 or 8 h under NH$_3$ flow of 50ml/min without air exposure, as reported in Ref. [4].

Crystalline phase was characterized using powder X-ray diffraction for the nitrided products dipped in silicone oil to prevent air exposure. X-ray absorption spectra of Fe and Co K-edges were measured in transmission mode at the beam line 9C in Photon Factory, in KEK. The spectrum was analyzed using the program REX2000 [5].

3 Results and Discussion

The nitrided products were mixture of nominal "α"-(Fe$_{1-x}$Co$_x$)$_{16}$N$_2$" and bcc-(Fe$_{1-x}$Co$_x$) alloy. Maximum yield in 42 wt% of the "α"-(Fe$_{1-x}$Co$_x$)$_{16}$N$_2$" was observed at x=0.03 in 8h of nitridation duration. However, the yield decreased by increasing Co content. The radial distributions were calculated by the Fourier transform of the EXAFS region for Fe and Co K-edges in the nitrided products. Bonding around Fe/Co atoms appeared at around 0.21 nm for the nitrided products at x=0.03 as shown in Figs. 1(a) and 1(c). Longer duration did not

change significantly the distribution around Fe/Co atom at x=0.03. However, the corresponding distance around Co increased to 0.225 nm for the 5% Co doped product, although there was not much change around Fe atom in the products as shown in Figs. 1(b) and 1(d). The peak shift and different distribution around Co atom at x=0.05 imply the appearance of partial phase decomposition from bct "α"-(Fe$_{1-x}$Co$_x$)$_{16}$N$_2$" to Co$_2$N having a hcp stacking.
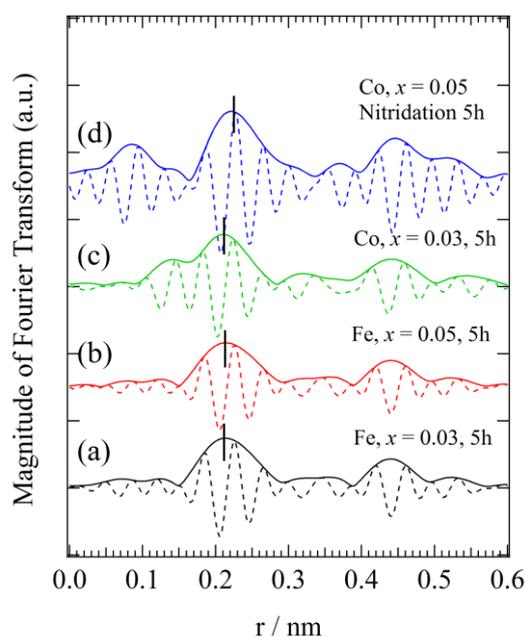

Fig. 1 Fourier transforms of the Fe K-edge spectra of the nitride products for nitidation duration of 5h, (a) at x=0.03, (b) x=0.05, and Co K-edge spectra (c) at x=0.03 and (d) at x=0.05. Thick lines were drawn as indicators for the distances from Fe/Co atom to metallic atoms in the products.

References
[1] S. Yamashita, *et al., J. Solid State Chem.*, **194**, 76 (2012).
[2] C. Kuhrt, *et al., J. Appl. Phys.*, **73**, 6588 (1993).
[3] H. Sadamura, *et al., J. Appl. Phys.*, **73**, 6731 (1993).
[4] Y. Masubuchi, *et al., J. Eur. Ceram. Soc.*, **31**, 2471 (2011).
[5] T. Taguchi, et al., *Phys. Scr.*, **T115**, 205, (2005).

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