High-resolution synchrotron X-ray powder diffraction study of lattice constants of Nd$_2$Fe$_{14}$B phase in Nd-Fe-B sintered magnets

S. Kobayashi$^{1,2}$, A. Martin-Cid$^{1,2}$, K. Toyoki$^{1,2}$, H. Okazaki$^{1,2}$, S. Hirosawa$^3$ and T. Nakamura$^{1,2}$

$^1$Japan Synchrotron Radiation Research Institute, 1-1-1 Kouto, Sayo, 679-5198, Japan.
$^2$Elements Strategy Initiative Center for Magnetic Materials, National Institute for Materials Science, Tsukuba 305-0047, Japan.

[Purpose]

The high-performance Nd-Fe-B magnets have been receiving considerable attention due to their outstanding magnetic properties. Owing to large magnetic moments of Fe atoms, the main phase of Nd$_2$Fe$_{14}$B exhibits large spontaneous volume magnetostriction of about 2%. In addition, the spontaneous magnetostriction is highly anisotropic as shown in Fig. 1. Andreev et al. have reported that the linear spontaneous magnetostrain along the $a$-axis ($\lambda_a$) is about 4.5 times larger than that along the $c$-axis ($\lambda_c$). However, Yang et al. have reported that $\lambda_a$ is only 1.7 times larger. It is very curious to find out the clear reason for this discrepancy, since magnetostriction should be intrinsic properties related to magnetization and magnetoelastic-coupling coefficients. In our previous study,$^{30}$ we showed the temperature dependences of the lattice constants for each constituent phase in a Nd-Fe-B-Cu anisotropic as-sintered magnet and found that they change differently from those expected for the pristine metal or compounds. This result indicates that lattice constants are influenced by some additional factors. In order to acquire a better understanding about the changes in the lattice constants, we have conducted high-resolution synchrotron XRD measurements in several kinds of samples.

[Experimental]

Isotropic and anisotropic Nd-Fe-B-Cu as-sintered magnets, their powdered samples, and powdered single crystals were used in this study. The preparation methods have been already reported.$^{3,4}$ The synchrotron XRD measurements of as-sintered magnets were conducted using rectangular rod-shaped samples ($0.2 \times 0.2 \times 5 \text{ mm}^3$). Synchrotron XRD profiles were collected at the BL02B2 beamline at SPring-8.

[Results]

Above $T_C$, the lattice constants of the Nd$_2$Fe$_{14}$B phase in as-sintered magnets, their powdered samples, and powdered single crystals showed a similar temperature variation. Lattice constants of all the samples exhibited a clear anomaly around the same temperature of $T_C \approx 580$ K and exhibited an invar-like expansion below $T_C$, which is similar to previous reports [see Fig. 1].$^{1,2}$ Interestingly, the behaviour of the lattice constants below $T_C$ was different, and the $a$-axis increased and $c$-axis decreased in the following order: the isotropic as-sintered magnet, anisotropic as-sintered magnet, their powdered samples, and powdered single crystals. In addition, a broadening of the diffraction peaks was observed for isotropic and anisotropic as-sintered magnets below $T_C$, while this broadening was negligibly small for powdered samples. The Williamson-Hall analysis clarified that the origin of the peak broadening was likely due to internal lattice strain in the sintered magnets. These results indicate that there exists an anisotropic stress applied to the Nd$_2$Fe$_{14}$B crystal grains in the sintered magnets. Our experimental results settled the problem of discrepancy in $\lambda_a/\lambda_c$.

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References