Effect of Magnetic field on crystal structure in antiferromagnetic NiO nanoparticles

Takayuki TAJIRI$^1,*$ and Masaki MITO$^2$

$^1$ Faculty of Science, Fukuoka University, 8-19-1 Nanakuma, Jonan-ku, Fukuoka 814-0180, Japan
$^2$ Kyushu Institute of Technology, 1-1 Sensui-cho, Tobata-ku, Kitakyushu-shi 804-8550, Japan

1 Introduction
Surface states of nanoparticles are changed by the development of the lattice strain owing to the existence of edges and defects at the surface of a particle as well as the crystallographic structure different from that of the bulk crystal. We investigated the crystal structure and magnetic properties of nanoparticles of an antiferromagnetic compound NiO with particle sizes ranging from 2.6 to 22 nm. The crystal structure and magnetic properties of NiO nanoparticles are sensitive to the particle size and have exhibited unique size dependences [1]. The magnetic properties of the NiO nanoparticles were explained by the core–shell model and exhibited large shell moment at surface of a nanoparticle. Kodama et al. calculated the equilibrium spin configurations in NiO nanoparticles, which resulted in 8-, 6-, or 4-sublattice spin ordering with decreasing particle size [2]. The size dependence of magnetic properties and crystal structure on NiO nanoparticles indicated an existence of strong correlation between spin configuration and crystallographic structure. It is expected that the change in spin configuration by apply of external magnetic field result in the change in the crystallographic structure. In this study, we investigated the correlation between spin configuration and crystal structure through X-ray diffraction measurements in the magnetic field.

2 Experiment
The NiO nanoparticles with particle size $d = 2.6$–$22$ nm were synthesized in the pores of mesoporous silica [1]. Powder XRD measurements were carried out using the a Debye-Scherrer camera at room temperature in external magnetic field up to 0.3 T. The incident X-ray energy was 16 keV and its wavelength was calibrated using the XRD pattern of the CeO$_2$ powder. Two facing NdFeB magnets were used to produce the external magnetic field. The magnetic field were changed by controlling the distance between the sample and NdFeB magnets [3]. The XRD patterns were analyzed to estimate the lattice constants by Rietveld analysis.

3 Results and Discussion
The crystallographic structure of the NiO bulk crystal is the so-called rock-salt structure that undergoes a transformation from the cubic symmetry to the rhombohedral one below the Néel temperature $T_N = 523$ K [4]. We observed the powder XRD patterns for the NiO nanoparticles with $d = 3.2$–$19.5$ nm in magnetic field up 0.3 T at 300 K. The XRD patterns of all NiO nanoparticles exhibited some broad Bragg peaks, which could be attributed to the rhombohedral distorted rock-salt structure in magnetic field up to 0.3 T. Fig. 1 shows magnetic field dependence of lattice constants of NiO nanoparticles with $d = 4.3$ and $11.7$ nm. The relative changes in lattice constants increased with decreasing particle size. These results indicated that the magnetostriction effects occurred in NiO nanoparticles and were enhanced with decreasing particle size. The NiO nanoparticles with $d < 10$ nm exhibited the pronounced change in lattice constants and magnetic properties [1]. The rhombohedral distortion $c/a$ for 4.3 nm increased with magnetic field and its relative change increased with decreasing particle size. The variation in $c/a$ led to the change in magnetic exchange interactions in NiO nanoparticles. The theoretical study of NiO nanoparticles concluded that the spin configuration of multiple sublattice structures changes with decreasing particle size, leading to an increase in the net magnetic moment [2]. The present results suggest that the pronounced changes in lattice constants for $d < 10$ nm were attributed to the increases in the multiple sublattice structures and net magnetic moment with decreasing particle size.

References

* tajiri@fukuoka-u.ac.jp