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Structural phase transition of spinel $NiCr_2O_4$ at low temperatures

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Introduction

$NiCr_2O_4$ with a normal spinel structure is known to show structural phase transition from cubic phase (space group: $Fd\bar{3}m$) to tetragonal one ($I4_1/amd$) at ~310 K because of Jahn-Teller effect on Ni^{2+} site. This compound shows magnetic ordering to ferromagnetism below T_C ~ 65 K. Very recently, Klemme et al reported another transition at ~30 K by heat capacity measurement [1]. After that, Tomiyasu et al reported that this transition is due to the change in magnetic structure by neutron and magnetization measurements [2].

In this study, we investigate the precise crystal structure of $NiCr_2O_4$ by high resolution x-ray powder diffraction measurement and discuss the correlation between magnetic and structural properties.

Experimental

The $NiCr_2O_4$ powder sample was prepared by heating the mixture of high purity NiO and Cr_2O_3 in air. The powder diffraction experiment was performed using high-resolution diffractometer installed at a beam line of BL-3A station. A wavelength of incident beam used was 1.600 Å. A flat Si(111) crystal analyzer was used in order to obtain the data with high angular resolution. The temperature dependence of the diffraction profiles of specific reflections were measured at temperatures between 12 K and 100 K using $2\theta/\theta$ scanning mode.

Results and discussion

Figure 1 shows the temperature dependence of powder diffraction profile in the 2θ range around 400 reflection, where the indices of Bragg reflections are based on the cubic structure. Above 70 K, the tetragonal structure is confirmed as previously reported [2]. However, the line width of 400 reflection becomes larger below 60 K and finally 400 reflection clearly splits into two peaks at the lower temperatures. We carefully checked the peak splitting for the other reflections, it is concluded that the crystal symmetry of $NiCr_2O_4$ below 60 K is orthorhombic.

Next, we determined the lattice constants for each temperature using a profile fitting technique. Figure 2 shows the temperature dependence of the lattice constants. The structural transition at ~ 60 K seems to be of second order because the lattice constants a and b change continuously. The transition temperature is almost the same as the magnetic ordering one, T_C, so that the crystal lattice of $NiCr_2O_4$ is strongly coupled with the magnetic ordering. On the other hand, the lattice constants show no evident anomaly at ~ 30 K.

The magnetic properties below T_C of $NiCr_2O_4$ has been discussed based on an assumption that the crystal structure is tetragonal so far. In the present study, we found that NCr_2O_4 has an orthorhombic structure below T_C, therefore it is necessary to reconstruct the magnetic structure and to reconsider the magnetic properties.

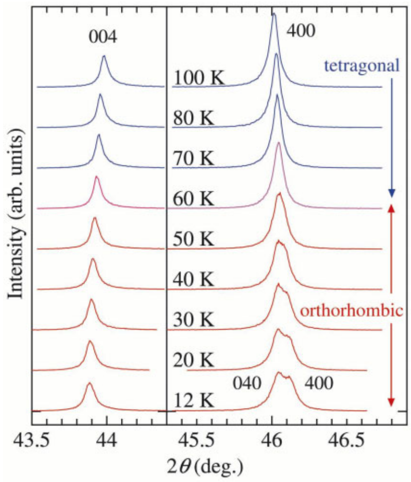

Fig. 1. Temperature dependence of powder X-ray diffraction patterns of $NiCr_2O_4$ on heating in the 2θ range around 400 reflection.

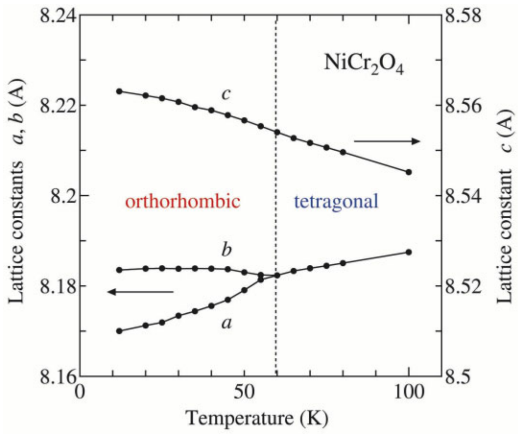

Fig. 2. Temperature dependence of lattice constants of $NiCr_2O_4$.

References

[1] S. Klemme et al., Phys. Chem. Miner. 29, 663 (2002).
[2] K. Tomiyasu et al., J. Phys. Soc. Jpn. 73, 2539 (2004).

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