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Crystal structure of ferrimagnetic phase of spinel compound $NiCr_2O_4$

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Introduction

$NiCr_2O_4$ has a tetragonally distorted spinel structure at room temperature and shows a unique ferrimagnetic ordering at T_C ~ 70 K. Recently, we reported that this compound exhibits a structural transition accompanied by the magnetic ordering, i.e., the crystal symmetry becomes orthorhombic below T_C [1]. However, the detail of the crystal structure of the ferrimagnetic phase has not been determined. The aim of this study is to determine the crystal structure of the ferrimagnetic phase of $NiC_{r2}O_4$ and to 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 experiments were performed using a high-resolution diffractometer installed at a beam line of BL-3A station. A wavelength of incident beam used was 0.900 Å. A flat Si(111) crystal analyzer was used in order to improve the angular resolution. The whole powder patterns were measured at 15, 40 and 100 K using $2\theta/\theta$ scanning mode.

Results and discussion

Figure 1(a) and 1(b) show the powder patterns of $NiCr_2O_4$ at 100 K and 15 K, respectively. The results of the Rietveld analysis using the data at 100 K, at which the crystal structure is known to be tetragonal with a space group $I4_1/amd$, are shown in Fig. 1(a) and Table 1(a). The overall quality of the fitting is fairly good. Next, in order to construct the structural model at 15 K, the crystal symmetry and the lattice constants are determined from the peak positions of Bragg reflections. All reflections can be indexed by the orthorhombic structure with the lattice constants of a ~ 8.171 Å, b ~ 8.184 Å and c ~ 8.563 Å. From the extinction rule, a space group *Fddd*, which is a subgroup of $I4_1/amd$, was assumed for a structural analysis. The results of the structural refinement are shown in Fig. 1(b) and Table 1(b), which show satisfactory results. The whole pattern at 40 K was also analyzed using the space group *Fddd*. The result is similar to that at 15 K except for the slight difference of the lattice constants.

From the present results, it is found that there are three kinds of bond distances between the neighbor Cr-Cr bonds for the ferrimagnetic phase. Compared to the magnetic structure obtained by Tomiyasu et al [2], the shortest Cr-Cr bond is corresponding to antiferromagnetic coupling, while the longest one is corresponding to ferromagnetic one. The distortion in the ferrimagnetic phase exhibits long range ordering, therefore there exists strong coupling between lattice and magnetism in $NiCr_2O_4$.

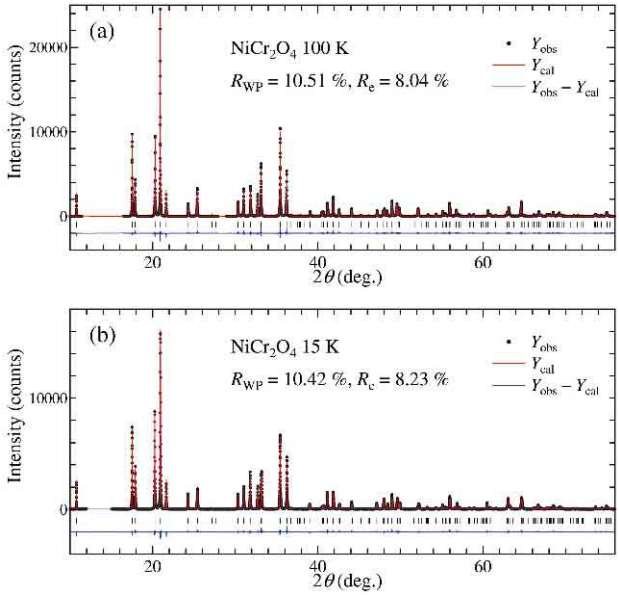

Fig. 1. X-ray diffraction patterns of $NiCr_2O_4$ at (a) 100 K and (b) 15 K and the Rietveld fit.

Table 1. Structural parameters obtained by Rietveld analysis at (a) 100 K and (b) 15 K.

(a) 100 K Space group $I4_1/amd$ (Origin choice 2)
a = 5.78951(3) Å, c = 8.54666(5) Å
R_{wp} = 10.51 %, R_B = 2.42 %, S = 1.31

atom	site	x	y	z	B (Å^2)
Ni	4*a*	1/8	1/8	1/8	0.040
Cr	8*d*	1/2	1/2	1/2	0.062
O	16*h*	0	0.0146(6)	0.2649(4)	0.052

(b) 15 K Space group *Fddd* (Origin choice 2)
a = 8.17161(6) Å, b = 8.18427(6) Å, c = 8.56287(5) Å
R_{wp} = 10.42 %, R_B = 2.94 %, S = 1.27

atom	site	x	y	z	B (Å^2)
Ni	8*a*	1/8	1/8	1/8	0.017
Cr	16*d*	1/2	1/2	1/2	0.055
O	32*h*	0.2576(4)	0.2554(4)	0.2669(2)	0.015

References

[1] H. Ishibashi et al., PF Activity Report 2004 #22 PART B, 156 (2005).
[2] K. Tomiyasu et al., J. Phys. Soc. Jpn. 73, 2539 (2004).

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