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Crystal distortion accompanied by ferrimagnetic transition in Laves phase $ErCo_2$

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Introduction

Laves compound $ErCo_2$ is known to show ferrimagnetic ordering below T_C ~ 32 K. At room temperature $ErCo_2$ has a cubic Laves structure with a space group $Fd3m$. Below T_C, rhombohedrally distorted structure was reported [1], however, the precise crystal structure of the ferrimagnetic phase has not been determined because of its small lattice distortion. Recently, it was found that the magnetic field induces the structural transition, i.e., the crystal symmetry increases to cubic in external magnetic field at 5 T [2]. In the present study, we investigate the detailed crystal structure under zero field at low temperatures by high resolution x-ray powder diffraction measurements to understand the mechanism of the magnetic field induced structural transition in $ErCo_2$.

Experimental

$ErCo_2$ compound was prepared by tetra-arc melting of stoichiometric amount of components followed by single-crystallization by Czochoralski method. The sample was carefully ground in acetone and fine powder was used for diffraction experiments. The powder diffraction experiments were performed using high-resolution diffractometer installed at a beam line of BL-3A station. A wavelength of incident beam used was 0.90 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 and whole powder patterns at 20 K and 40 K were measured.

Results and Discussion

Figure 1 shows the temperature dependence of powder diffraction pattern in the 2θ range around 222 and 440 reflections, where the indices of Bragg reflections are based on the cubic structure. The structural transition is clearly observed from cubic phase to distorted one at ~32.5 K, which is the same temperature as the ferrimagnetic ordering one. From Fig. 1, the Bragg peaks for both 222 and 440 reflections split into two peaks below the transition temperature, therefore the crystal symmetry is considered to be rhombohedral. It is noted that there exist two phases, the cubic phase and the distorted one, between 32.0 and 32.5 K, therefore the phase transition is of first order.

In order to determine the crystal system and the lattice constant below the transition temperature, we carefully checked the peak splitting using the whole powder pattern

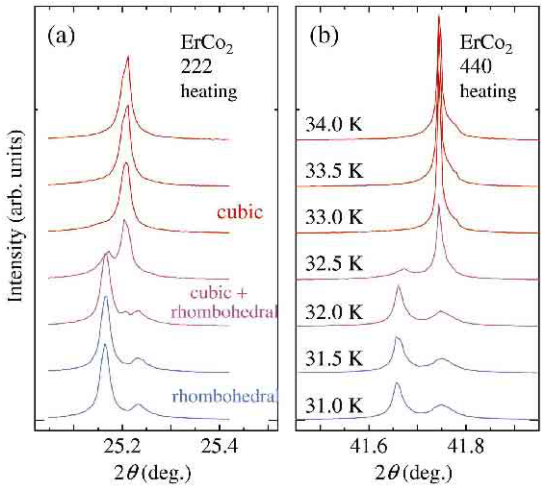

Fig. 1. Temperature dependence of powder x-ray diffraction patterns of $ErCo_2$ on heating in the 2θ range around (a) 222 and (b) 440 reflections.

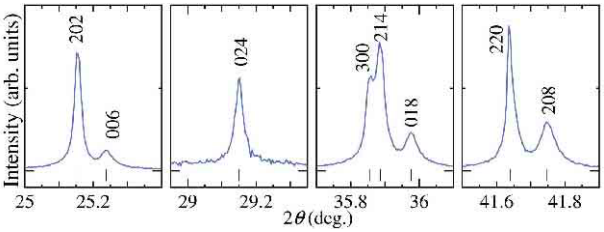

Fig. 2. X-ray diffraction pattern at 20 K. The indices are based on the rhombohedral symmetry with the lattice constant of a = 5.0605 Å and c = 12.351 Å.

at 20 K. As the result, all Bragg peaks can be indexed by a rhombohedral symmetry with the lattice constant of a = 5.0605 Å and c = 12.351 Å. The result of the indices is shown in Fig. 2. The rhombohedral symmetry implies that the lattice distorts a [111] direction, which is consistent with the easy direction of magnetization. The detailed structural analysis is now in progress.

References

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