

表題: 高温中性子粉末回折による  $\text{CaYAlO}_4$  の結晶構造解析  
Crystal structure analysis of  $\text{CaYAlO}_4$  by high-temperature neutron diffraction

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### 1. Introduction

$\text{K}_2\text{NiF}_4$ -type structure  $\text{ABCO}_4$  ( $A = \text{Ca, Sr, Ba}$ ;  $B =$  rare earth;  $M = \text{Al, Ga}$ ) is candidate for applications such as substrate and electrode materials. Crystal structure of  $\text{CaYAlO}_4$  has not been studied at high temperature by neutron diffraction so far. In the present work, we have investigated the crystal structure of  $\text{CaYAlO}_4$  by high-temperature neutron powder diffraction.

### 2. Experimental

$\text{CaYAlO}_4$  material was prepared by solid-state reactions.  $\text{CaYAlO}_4$  was prepared with stoichiometric mixtures of the  $\text{CaCO}_3$ ,  $\text{Y}_2\text{O}_3$ ,  $\text{Al}_2\text{O}_3$ , which were mixed with ethanol in an agate pot and calcined at 1073 K for 8 h in air. The calcined powder was then milled again. After a uniaxial pressing at 50 kPa, the disk was sintered in air at 1673 K for 3 h. The phase purity of  $\text{CaYAlO}_4$  was confirmed by X-ray diffraction measurements.

Neutron diffraction experiments were carried out on the Echidna high-resolution powder diffractometer at the OPAL reactor in Sydney, Australia. The neutron wavelength was 1.6602 Å, calibrated against a standard  $\text{Al}_2\text{O}_3$  sample. The data were collected in the temperature range from 298K to 1473K. The resulting diffraction data were analyzed by the Rietveld method with RIETAN-FP.

### 3. Result and Discussion

Rietveld analysis of the  $\text{CaYAlO}_4$  solid solution was carried out by the tetragonal structure with the  $I4/mmm$  space group at 298-1473 K. Figure 1 shows the Rietveld pattern of  $\text{CaYAlO}_4$  at room temperature. The reliability factors were  $R_{wp}=7.01\%$ ,  $R_B=2.67\%$ , and  $R_F=1.81\%$ . Phase transition was not observed at 298K to 1473K. Unit cell parameters were  $a = b$  3.6420(1)Å,  $c = 11.8919(5)$ Å. Unit cell parameter increased with increasing temperature.

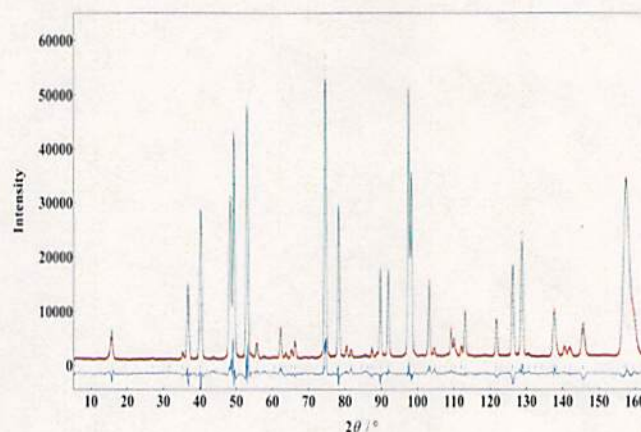


Fig. 1 Rietveld refinements of the neutron powder diffraction patterns of  $\text{CaYAlO}_4$  at 298 K.

### Acknowledgements

The (Type of experiment) experiment was performed by using (Instrument name) at (Facility), (Country), which was transferred from (Instrument at JRR-3) with the approval of Institute for Solid State Physics, The University of Tokyo (proposal no. #####), Japan Atomic Energy Agency, Tokai, Japan.