

Structural investigation of novel AA'BO₄-type mixed conductors

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Introduction

K₂NiF₄-type structured oxides AA'BO₄ (A = Ca, Sr, Ba; A' = rare earths; B = Al, Ga) are candidates for applications such as substrate and electrode materials. Crystal structure of ErCaAlO₄ has not been studied at high temperature by neutron diffraction yet. In the present work, we have investigated the crystal structure of ErCaAlO₄ by high-temperature neutron powder diffraction.

Experimental

ErCaAlO₄ material was prepared by solid-state reactions. ErCaAlO₄ was prepared with stoichiometric mixtures of the CaCO₃, Er₂O₃ and Al₂O₃, which were mixed with ethanol in an agate mortar and calcined at 800 °C for 8 h in air. The calcined powder was then milled again. After a uniaxial pressing at 50 MPa, the disk was sintered in air at 1400 °C for 3 h. The phase purity of ErCaAlO₄ was confirmed by X-ray powder diffraction measurements. Neutron diffraction experiments were carried out by the Echidna high-resolution powder diffractometer at the OPAL reactor of ANSTO in Sydney, Australia. The neutron wavelength was 1.6602 Å. The neutron diffraction data of ErCaAlO₄ were collected in the temperature range from 22 °C to 1473 °C. The diffraction data were analyzed by the Rietveld method with RIETAN-FP.

Result and Discussion

Rietveld analysis of ErCaAlO₄ solid solution was carried out by the K₂NiF₄-type structure with the tetragonal I₄/mmm symmetry from 298 to 1473 K. Figure 1 shows the Rietveld pattern of ErCaAlO₄ at 298 K. The reliability factors were R_p=3.03%, R_{wp}=3.93%, R_B=2.67%, and G_{oF}=3.53. Phase transition was not observed between 22 °C and 1473 °C. Refined

unit-cell parameters were $a = 3.64118(4)$ Å and $c = 11.8478(2)$ Å. Unit cell parameter of ErCaAlO₄ increased with increasing temperature.

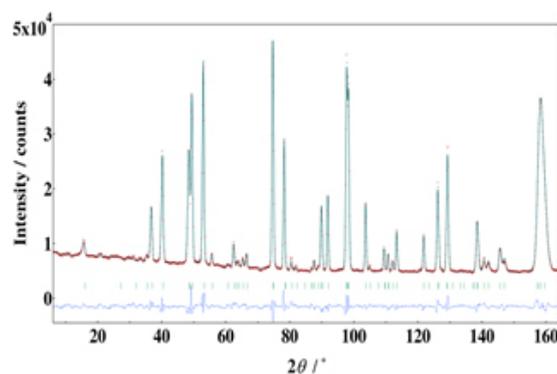


Fig. 1. Rietveld pattern of the neutron powder diffraction data of ErCaAlO₄ at 22 °C.