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Phase Transition of $KTiOPO_4$?

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Introduction

KTP ($KTiOPO_4$) is a well-known nonlinear optical material. The phase transition from ferroelectric phase (Space group: $Pna2_1$) to paraelectric phase (Space group: *Pnan*) at about 1207K was reported using SHG method[1], but the exact temperature depends on variations in the growth condition.[2] No crystallographic studies have been reported on the phase transition of KTP based on diffraction experiments at high temperatures. In this study, we measured the synchrotron powder diffraction data of KTP around 1200K to investigate the phase transition.

Experimental

$KTiOPO_4$ sample was prepared by solid state reactions. K_2CO_3, TiO_2, and $NH_4H_2PO_4$ were used as starting materials. They were mixed and ground with an agate mortar and by planetary ball milling. The mixture was sintered at 1273K for 3 h in air.

Synchrotron x-ray powder diffraction data were collected using the multi-detector diffractometer installed at BL-$4B_2$ of Photon Factory, KEK, Tsukuba, Japan. The wavelength was determined to be λ=1.20645Å Diffraction data were collected at 1123 K and 1236 K in the 2θ range from 10° to 155° in the step interval of 0.005° in 2θ using a furnace with molybdenum silicide heaters.[2, 3] The diffraction data were analyzed by the Rietveld method with a computer program RIETAN-2000.

Results and discussion

All the reflections at lower angle of powder diffraction data at 1123K was indexed by $Pna2_1$ KTP and $P4_2/mnm$ TiO_2, impurity. The unit-cell parameters were determined by the Rietveld analysis (Table.1). The unit-cell parameters *a, b* and *c* at 1123 K were larger than those at room temperature.[4]

Figure 1 shows synchrotron x-ray powder diffraction patterns of KTP at (a) 1123K and (b) 1236K. Diffraction patterns were similar between these temperatures, suggesting no phase transition.

Table.1: Unit-cell parameters of KTP at 1123K

a (Å)	***b*** (Å)	***c*** (Å)	$\alpha=\beta=\gamma$(°)
12.9426(2)	6.4805(1)	10.5531(2)	90

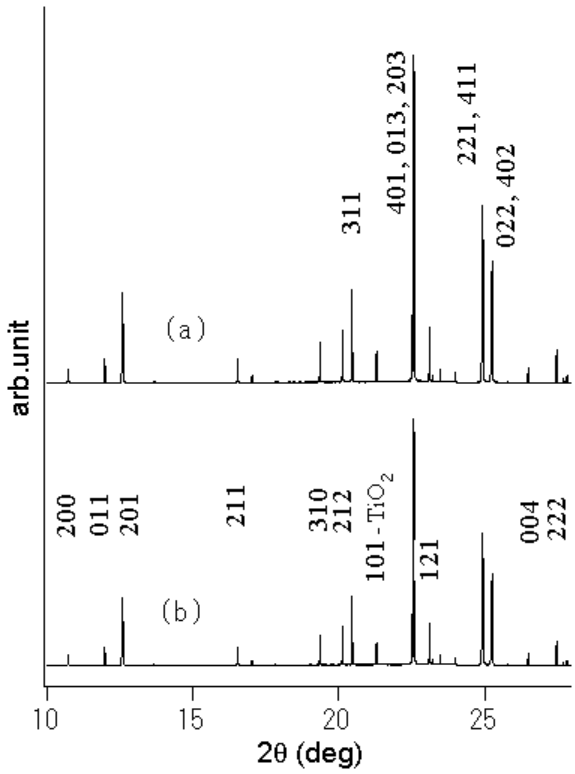

Fig. 1: Synchrotron x-ray powder diffraction patterns of KTP measured at (a) 1123K and (b) 1236K.

References

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