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High-temperature synchrotron X-ray powder diffraction study of the tetragonal-cubic phase transition of 10 mol% Yb_2O_3-Bi_2O_3

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Introduction

The δ phase of Bi_2O_3 is known as the highest oxide-ion conductor. But this phase is stable only between 723°C and 825°C. To stabilize the δ phase to room temperature, doping of rare earth oxide is necessary. Many researchers have studied the doping effect. However the temperature dependence of lattice parameters and the mechanism of phase transition between tetragonal and cubic phase have not been studied well. In this study we investigate the temperature dependence of powder diffraction profile and the mechanism of the phase transition between tetragonal and cubic phases of 10mol% Yb_2O_3 doped Bi_2O_3.

Experiments and results

$(Bi_2O_3)_{0.9}(Yb_2O_3)_{0.1}$ sample was prepared by conventional solid-state reaction method as follows. High-purity Bi_2O_3 (99.9%) and Yb_2O_3 (99.9%) were mixed with ethanol in an agate mortar and fired at 750°C for 12 h. Samples were then ground in an alumina mortar and pressed into pellets under a pressure of 200 MPa, followed by sintering at 850°C for 12 h, then cooled slowly for three days. Phase purity was confirmed by X-ray powder diffraction using Cu Kα radiation.

To investigate the phase transition we performed synchrotron X-ray powder diffraction experiments for $(Bi_{0.9}Yb_{0.1})_2O_3$ at the beam line BL-3A at the Photon Factory, High Energy Accelerator Research Organization. A monochromatized 0.99931(6) Å X-ray was used for high-temperature diffraction experiments. To improve the angular resolution a Si (111) analyzer crystal was installed between the sample and the scintillation counter. The angular resolution $\Delta d/d$ was estimated to be 0.0002 from the peak width for the standard CeO_2 powders where d is the lattice spacing.

Fig.1 shows the temperature dependence of synchrotron X-ray powder diffraction profile for 002 and 220 reflections on heating (a) and on cooling (b). On heating only 002 and 220 peaks were observed from 100 to 675°C, indicating a single tetragonal phase. At 685°C, there appeared three peaks, indicating the coexistence of the tetragonal and cubic phases. Thus, the transition is of first order. The $(Bi_2O_3)_{0.9}(Yb_2O_3)_{0.1}$ was cubic phase between 695 and 740°C and between 740 and 600°C on heating and on cooling, respectively. The tetragonal phase transforms into the cubic form between 675 and 695°C on heating, while the inverse cubic-to-tetragonal transformation occurred between 600 and 575°C on cooling. This indicates a thermal hysteriesis of about 100°C. Therefore, the tetragonal-cubic phase transition is of first order.

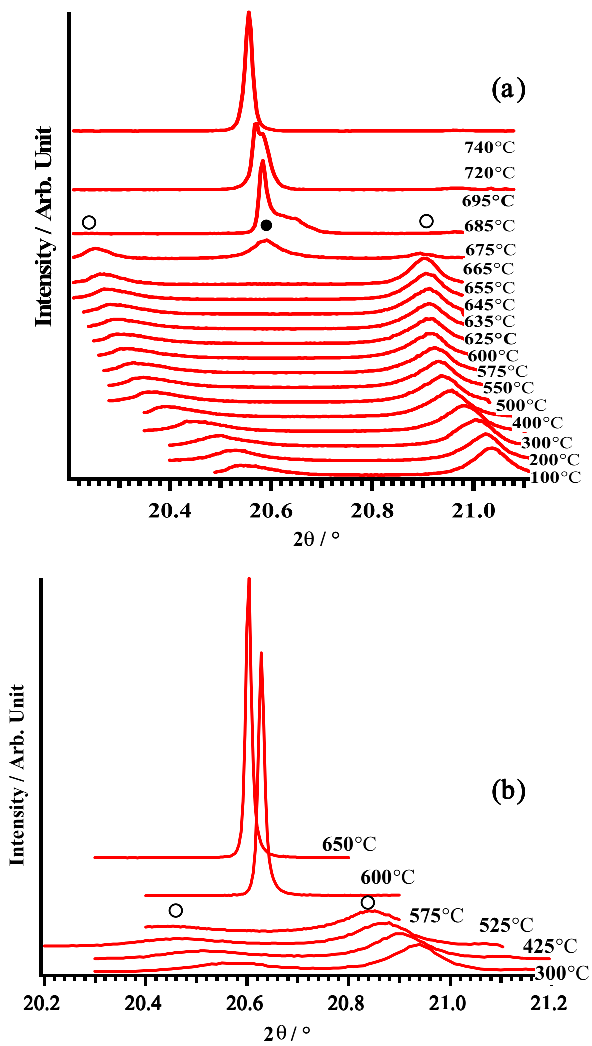

Fig.1. Temperature dependence of synchrotron X-ray powder diffraction profile for 002 and 220 reflections on heating (a) and cooling (b).

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