

Phase Transition of Hexagonal BaTiO₃

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1. Introduction

Hexagonal BaTiO₃ undergoes successive phase transitions at 222K and 74K from the hexagonal phase I (room temperature phase), to phase II (intermediate phase) and phase III (the lowest ferroelectric phase). The characteristics of low temperature phases are not clear yet, even the unit cell of phase III. We are studying the structures of phase II and phase III by using neutron powder diffraction, high resolution synchrotron powder diffraction and single crystal experiments at laboratory low temperature photograph method.

The purpose of the present work is to study the symmetry of the unit cell of h-BaTiO₃ at low temperature phases and measure the lattice parameters as a function of temperature.

2. Experimental

X-ray diffraction experiments were performed at the Crystal Structure Analysis beam-line (BL02B1) in SPring-8. A powder sample of h-BaTiO₃ was prepared. For the room temperature experiments, it was mounted on a glass plate holder which was settled on a sample-spindle. For low temperature experiments, it was mounted on an Al plate and put in a cryostat.

Double monochromators with Si 111 or Si 311 were used. First, we tuned the counter system for X-ray energies from 5keV to 70keV by using a Bragg reflection of the sample. In order to change the X-ray energy, we developed a communication program to the host-computer of the monochromator so that the fine tuning of the monochromator became very easy. Then, we tested the cryostat. After the tune-up of the cryostat, the stability of temperature became less than 0.1K. Ring current during the experiments was about 19mA. For the high resolution experiments, we used an analyzer Si 220 crystal.

3. Results and Discussion

Fig. 1 shows an observed width(FWHM) as a function of the diffraction angle. The X-ray energy used was 14.26keV(0.869Å). The best resolution we have obtained was $\Delta 2\theta = 0.0085^\circ$ at $2\theta = 24^\circ$.

We determined the symmetry of phase II and III of h-BT. The unit cell and the space group of phase II were confirmed to be the orthorhombic and C222₁. The symmetry in phase III is newly determined as a monoclinic with the deformation of the γ -angle(about 0.05degree) by this experiment. The most possible symmetry in phase III is C112₁, or equivalently P112₁ as a crystallographic conventional unit cell. In Fig.2, we show the typical examples of the powder diffraction profiles as a function of temperature.

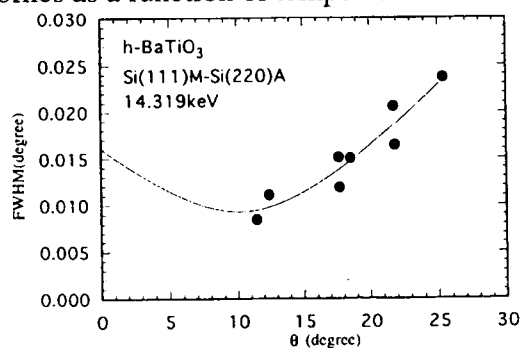


Fig.1 FWHM of powder diffraction profile as a function of diffraction angle

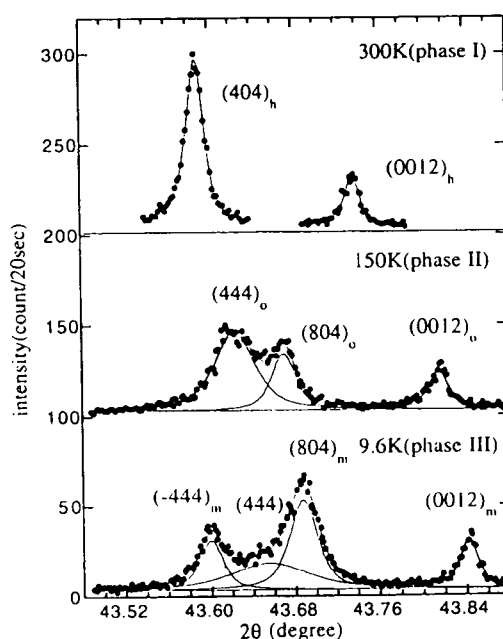


Fig.2 Powder diffraction in Phase I, II and III.