Phase Transition of Hexagonal $BaTiO_3$

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1. Introduction

Hexagonal $BaTiO_3$ undergoes successive phase transitions at 222K and 74K from the hexagonal Phase I, to Phase II (intermediate phase) and Phase III. Only known in Phase III is that this phase is ferroelectric. The purpose of the present experiment is to make clear the symmetry and the unit cell of Phase III. In addition, we developed the technique to do the low temperature powder diffraction experiment at BL02B1.

2. Experimental

X-ray diffraction experiments were performed at the Crystal Structure Analysis beamline (BL02B1) in SPring-8. A powder sample of *h*-$BaTiO_3$ was mounted on an Al -plate and was put in a cryostat for the low temperature experiments. The lowest temperature we could achieve was 9K and the stability of temperature was better than 0.1K. Double monochromators of Si 111 were used. We used an analyzer Si 220 crystal to obtain high resolution. The wave length was 0.86519A.

3. Results and Discussion

As was mentioned in the last report (1997B0027-ND-np), we could obtained very high resolution powder diffraction profiles. The best record of the diffraction width of the powder diffraction of *h*-$BaTiO_3$ was 0.0085 degree. This high resolution was the key point to solve the symmetry of the low temperature phases of *h*-$BaTiO_3$ since the distortion of the lattice was one magnitude smaller than those of the phase transitions in the ordinal materials.

The final conclusion was as follows: Phase I is a hexagonal phase, and phase II has a C-based orthorhombic cell. In Phase III, the orthorhombic cell of Phase II distorts and has a C-based monoclinic cell with the γ-angle distortion. Such a cell is usually transformed to a primitive cell. Fig. 1 shows the characteristic distortion associated with the phase transition referred to the primitive unit cell, as a function of the temperature. Upper figure shows the difference of the two principle axes and the lower one is the angle distortion. The difference of the length of axes is only 0.005A and the angle distortion is about 0.1 degree. In the figure, we also show the result of the high resolution single crystal experiments at the laboratory system. This result is assumed the lattice form determined by the present powder experiment. As is well known, a single crystal experiment gives much better resolution than that of the powder diffraction experiments, partially due to the intensity problem. Both results give a comparable resolution. That is, the powder diffraction at BL02B1 gives the comparable resolution of the single crystal high resolution experiment at the laboratory system, and obviously 20 times better resolution than that of the laboratory powder experiments.

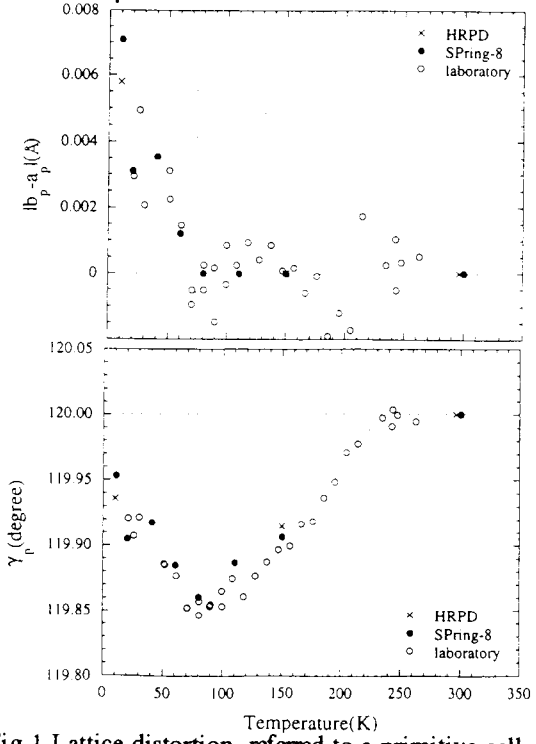

Fig.1 Lattice distortion referred to a primitive cell.