

## X-Ray Diffraction Study on the Phase Transitions of Barium Titanate

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Structural phase transitions in as-grown single crystal of BaTiO<sub>3</sub> were studied by X-ray precession method in the temperature range between 420 K and 90 K. It was found that high temperature cubic phase, designated here as cubic I, is transformed into the room temperature phase (RTP at T<sub>1</sub>=403 K), and further into the low temperature phase (LTP at T<sub>2</sub>=278 K), in both of which closely related two structures coexist to form domains with a shape of multi-domain 'hybrid' structure. In RTP the coexisting structures are tetragonal I and monoclinic I and in the LTP tetragonal II and monoclinic II. On the other hand, the lowest temperature phase (below T<sub>3</sub>=183 K) is in a single domain of a tetragonal III form. These observations are in disagreement with the phase transition sequence, proposed by previous studies, cubic→tetragonal→orthorhombic→rhombohedral. The lattice constants of the tetragonal I form are a<sub>TI</sub>=0.4009(10) nm and c<sub>TI</sub>=0.4048(10) nm, and those of the monoclinic I form are a<sub>MI</sub>=0.4059(10), b<sub>MI</sub>=0.4009(10), c<sub>MI</sub>=0.5700(10) nm and β<sub>MI</sub>=135.33(10)° at room temperature. Those of the tetragonal II form are a<sub>TII</sub>=0.4027(10) and c<sub>TII</sub>=0.3996(10) nm, and those of the monoclinic II form are a<sub>MII</sub>=0.3994(10), b<sub>MII</sub>=0.4027(10), c<sub>MII</sub>=0.5678(10) nm and β<sub>MII</sub>=134.77(10)° at 233 K. Evolution and crystallographic relationship of the four phases forming the multi-domain 'hybrid' structures are presented.

**Keywords:** BaTiO<sub>3</sub>, phase transitions, 'hybrid' structure