Structural analysis and Phase transitions in $BaTiO_3$

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1 Objective

To obtain the X-ray diffraction pattern of $BaTiO_3$ and realise the structural phase transitions.

2 Introduction

X-ray diffraction crystallography commonly used by crystallographers to study crystals. The incident X-ray is diffracted and the diffracted beam contains the information of the crystal. The diffracted angle gives the information of crystal structure and Intensity gives the electron density at the region.

3 Theory: X-ray diffraction

When an X-ray of wavelength (λ) is made to incident on a crystal, if the wavelength is smaller than the lattice parameter diffracted beams are obtained in a direction slightly different from that of incident beam is obtained. The diffracted beams upon reflection from different planes of the crytal interfere constructively and give diffraction pattern. Being an electromagnetic wave, X-ray undergoes an phase change under diffraction written as,

$$F = \sum_G \int n(\mathbf{r}) e^{i(\mathbf{k}-\mathbf{k}').\mathbf{r}} \, \mathrm{d}V$$

Local electron concentration in the crystal,

$$n(\mathbf{r}) = \sum_G n_G e^{i\mathbf{G}.\mathbf{r}}$$

$F = \sum_G \int n_G e^{i\mathbf{G}.\mathbf{r}} e^{i(-\Delta\mathbf{k}).\mathbf{r}} \, \mathrm{d}V$ Where $\Delta\mathbf{k} = \mathbf{k}' - \mathbf{k}$.
The scattering amplitude becomes negligibly small when the phase difference in

wavevector differs significantly from the reciprocal lattice vector. This yields, $\Delta\mathbf{k} = \mathbf{G} \implies \mathbf{k} + \mathbf{G} = \mathbf{k}'$ In elastic collision, kinetic energy is conserve,

$$k' = k$$

yields, $2\mathbf{kG} = \mathbf{G}^2$.G is a reciprocal lattice vector,$G = h\mathbf{b_1} + k\mathbf{b_2} + l\mathbf{b_3}$ comes out as

$$2d\sin\theta = n\lambda$$

Where d is the lattice spacing between the crystal planes.

4 Instrument: X-ray Diffractometer

X-ray diffractometer instrument has a x-ray source emitted from Coolidge's tube and and made to fall on the crystal loaded in the sample holder (powder samples). A detector is kept at angle (θ) opposite to the the incident beam. The goniometer aids in the movement of the detector and source along the circular scale. The detector pulses (I) are counted in synchronisation with the movement of goniometer (θ). The sample table is provided with the rotator such that the

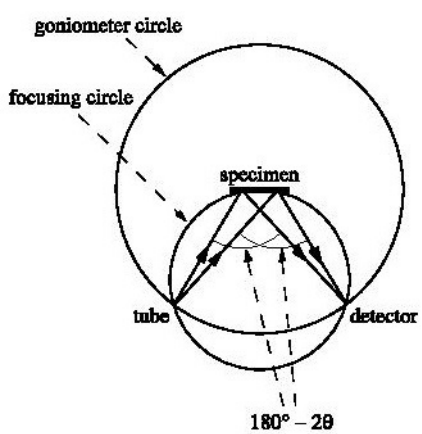

Figure 1: Scheme of a Diffractometer.

pattern is taken with different orientations. The measurements are collected in the computer interfaced with the instrument. The lattice parameter d(hkl) can be dtermined by the braggs formula with different orientation. The peaks are identified using the JCPDS data and the structure is determined.

5 Results and Analysis

- The Intensity (scattering amplitude) of the diffracted beam gives the information of the structure factor from where the structure is determined.

- The lattice parameters of $BaTiO_3$ at different temperatures are:
  At T=300K, a=b=3.993055Å, c=4.032882 Å(Tetrogonal phase)
  At T=260K, a=3.985320 Å, b=5.670149 Åand c=5.686303 Å(Orthorhombic Phase).
  At T=150K, a=b=5.656044 Å, and c=6.948219 Å(Rhombohedral Phase).
  Rhombohedral $\xrightarrow{Above 260K}$ Orthorhombic $\xrightarrow{Above 300K}$ Tetrogonal phase

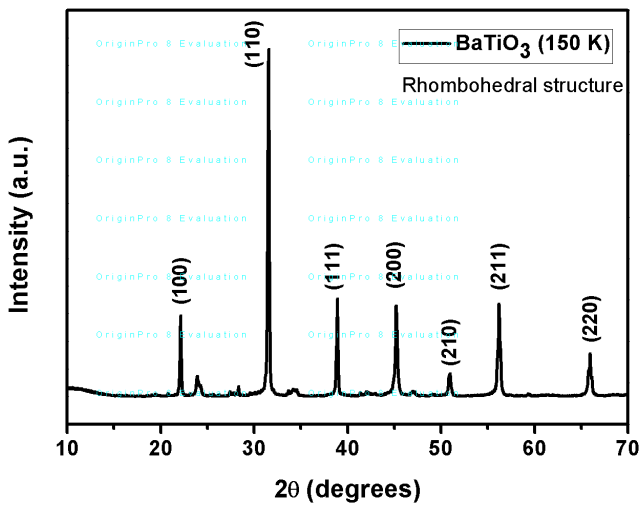

Figure 2: Diffraction pattern of $BaTiO_3$ at 150K

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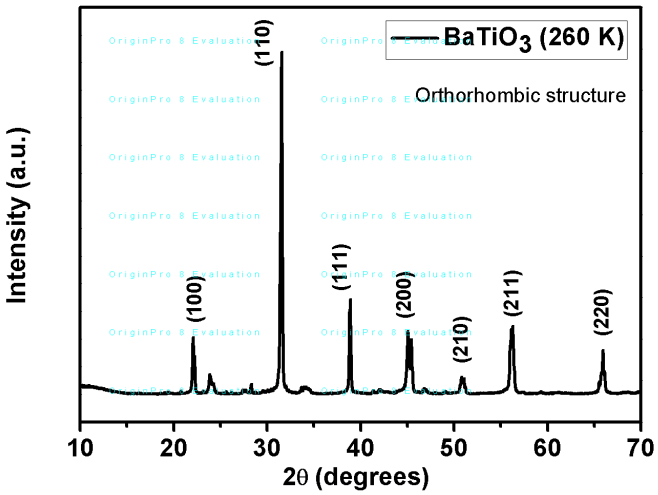

Figure 3: Diffraction pattern of $BaTiO_3$ at 260K

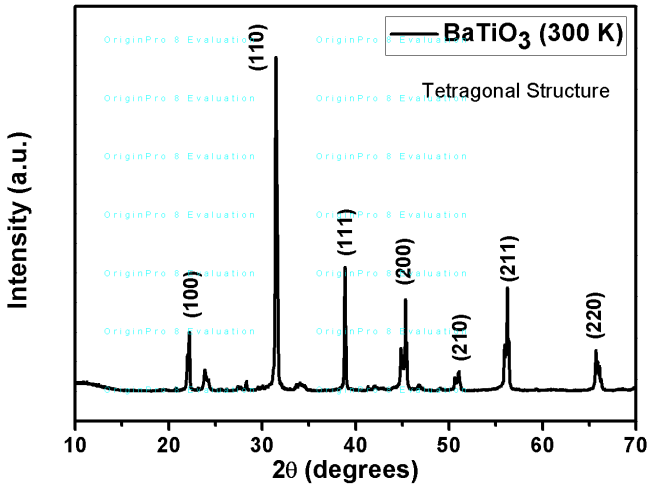

Figure 4: Diffraction pattern of $BaTiO_3$ at 300K.