

[View on rigaku.com](https://www.rigaku.com)

B-XRD1149 - Evaluation of barium titanate polymorphs by Rietveld analysis

Introduction

Barium titanate (BaTiO_3) is a representative ferroelectric material, used in capacitors and electronic components such as pyroelectrics and piezoelectrics. Barium titanate exists as tetragonal and cubic systems at room temperature. The mass fractions of these two phases affect its permittivity. In addition, the c/a ratio of the tetragonal phase also affects permittivity. Therefore, it is important to determine the mass fractions of the polymorphs and lattice constants to control the permittivity of barium titanate. Rietveld analysis allows you to easily calculate mass fractions and lattice constants based on the X-ray diffraction pattern. In this example, the X-ray diffraction pattern was obtained using a compact X-ray diffractometer, equipped with the high-resolution and high-speed one-dimensional detector D/teX Ultra250. We evaluated mass fractions and lattice constants of barium titanate by Rietveld analysis.

Measurements and results

We used a commercially available barium titanate powder (FUJIFILM Wako Pure Chemical Corporation) for the measurement. Rietveld analysis was performed using integrated X-ray analysis software SmartLab Studio II. Results of the Rietveld analysis are shown in Figure 1, Table 1 and 2. Mass fractions (Table 1) and lattice constants (Table 2) can be obtained simultaneously in a single Rietveld analysis. Additionally, it is possible to easily analyze multiple data sets all at once using an analysis template.

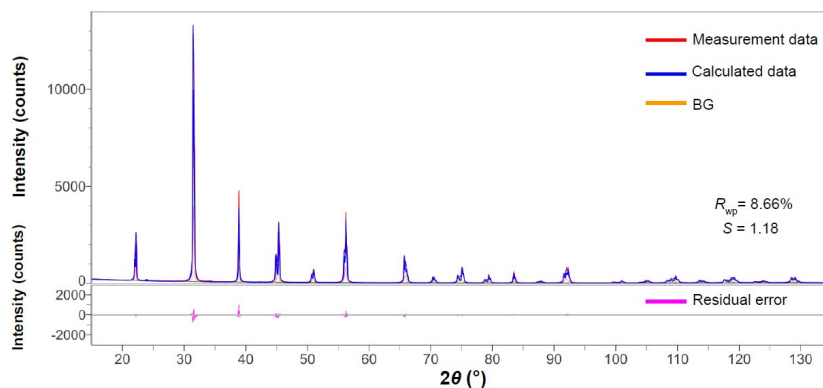


Figure 1: Profile fitting results using Rietveld analysis for the barium titanate sample

Table 1: Quantitative results of the barium titanate powder sample

Crystal phase	Mass fraction (mass%)
BaTiO_3 (tetragonal)	76.1

BaTiO ₃ (cubic)	22.8
BaCO ₃	1.12

Table 2: Lattice constants and the c/a ratio of the tetragonal barium titanate

a (Å)	c (Å)	c/a ratio
3.99525	4.03494	1.009934

Related products



MiniFlex

New sixth-generation general purpose benchtop XRD system for phase i.d and phase quantification



MiniFlex XpC

Compact X-ray diffractometer for quality control of materials that is easy to use and is ideal for routine work



SmartLab

Advanced state-of-the-art high-resolution XRD system powered by Guidance expert system software



SmartLab SE

Highly versatile multipurpose X-ray diffractometer with built-in intelligent guidance



SmartLab Studio II

Windows-based software suite for Rigaku's X-ray diffractometers