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$BaBi_4Ti_4O_{15}$: Synthesis and characterization

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Abstract

Aurivillius oxide $BaBi_4T_{i4}O_{15}$ (BBT) has been used in the applied nanomaterials technology. The ferroelectric materials properties expected to alternative solutions for computer memories, makes ferroelectric nonvolatile memories very attractive. The aim of this research is to determine structure and surface morphology of $BaBi_4Ti_4O_{15}$ synthesis. The solid state reaction method is used in this research. In the solid state reaction the temperature of 800 to 1100 ^oC is applied for 24 hours. X-ray diffraction powder and SEM-EDAX ((Scanning Electron Microscope-Energy Dispersive Analysis of X-rays) are also used to determine the crystal structure. The results are in excellent agreement with the data that reported in PDF (Powder Diffraction File) Number 84-1750 (orthorhombic). The surface analysis of $BaBi_4Ti_4O_{15}$ showed that the crystals are polycrystalline with the size of 219.967 Å. Qualitative analyses using EDAX showed that Ba:Bi ratio in the crystal is 1:4.

Keywords: BBT, solid state reaction, aurivillius, orthorhombic, polycrystalline

Introduction

Ferroelectric materials have innumerable properties related to their spontaneous polarization, for instance, pyro and piezoelectricity, which are used for various sensors and actuators. The use of ferroelectric thin films brings not only the additional advantage of reduced weight and size, but it allows the fabrication of integrated devices which involve switching of the polarization between the two thermodynamically stable states. The development of sophisticated film-synthesis methods providing high-quality films, together with presently existing efforts to find new or alternative solutions for computer memories, makes ferroelectric nonvolatile memories very attractive. Simple perovskite ferroelectric films (such as PZT) on platinized silicon substrates exhibit high polarization fatigue. This problem could be overcome to some extent by replacing the Pt electrodes with conducting oxide electrodes or by replacing PZT with Bi based layer-structured ferroelectric oxides, which are known to be free of polarization fatigue up to 10^{12} cycles of polarization. These Bi-based layer-structured ferroelectric oxides belong to the Aurivillius family and can be described by the general formula $(Bi_2O_2)^{++}(A_{n-1}B_nO_{3n+1})^{--}$ (Satyalakshmi *et al.*, 1998).

One interesting feature of the Aurivillius phases resides in the compositional flexibility of the perovskite blocks which allows to incorporate various cations such as Na^+, K^+, Ca^{2+}, Sr^{2+}, Ba^{2+}, Pb^{2+}, Bi^{3+} or Ln^{3+} for the A-site and Fe^{3+}, Cr^{3+}, Ti^{4+}, Nb^{5+} or W^{6+} for the B-site. It is thus possible to modify the ferroelectric properties according to the chemical composition. As an illustration, the majority of the Aurivillius oxides where A=Ba have a relax or type ferroelectric behavior to the difference of their analogues where A=Sr, Ca and Pb. Although this phenomenon was observed since many years, its structural origin is not yet clearly elucidated.

There is a considerable interest in replacing the current generation of thin film ferroelectrics, based on the perovskite (PZT), both from an environmental view and to improve performance. These Aurivillius oxides do not contain any of the toxic heavy metal, lead, and they also display superior fatigue-free behavior and lower coercive fields compared to PZT (Kennedy et al., 2003).

Very little is known about the information structure of the n=4 oxide. In the present work, we have determined the structure of the BBT. We had also to find out information about surface morphology of BBT.

Materials and Methods

$BaBi_4Ti_4O_{15}$ was prepared by the solid state reaction of $BaCO_3$, Bi_2O_3 and TiO_2 at 800, 850, 900, 950, 1000, 1050 and 1100 ^oC for 24 hours. Each with regrinding after each heating step. The structure and morphologhy sample were determined used by X-ray diffraction powder and SEM-EDAX. Refinement structure using Le bail program from Rietica method.

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Results and Discussion

Preliminary X-ray diffraction data, recorded using Cu Kα radiation did not show any evidence of impurity phases. The observed pattern was in excellent agreement with that reported for orthorombic $BaBi_4Ti_4O_{15}$. Structural parameters (Table 1) were refined by the Le Bail method with the program Rietica.

Table 1 Pameter of BBT cell refinment with Le Bail method.

Crystal structure	*A2₁am* (orthorombic at room temperature)	
Cell parameters	BBT	
	PDF Data base	Le Baile calculated method
A (Å)	5.4309	5.4331(1)
b (Å)	5.4554	5.4565(1)
c (Å)	49.4921	49.5031(1)
R_p	4.35	4.39
R_{wp}	5.32	6.07

The difractogram from observation was compared with difractogran from PDF (Powder Diffraction File) software. The difractogram produce similiar peaks to PDF Number 35-0757 .

Plot the observed and calculated data was showed in Figure 1.

Particel size from BBT is 219.967 Å calculated with Scherrer equation:

$$t = \frac{0{,}92\lambda}{\beta}\cos\theta$$

With, t = crystal size
λ = wave length
β = peak width-full width at half maximum
θ = diffraction angle.

The surface analysis of $BaBi_4Ti_4O_{15}$ using SEM (Scanning Electron Microscope) and qualitative analyses of composition element using EDAX (energy-dispersive analysis of X-rays).

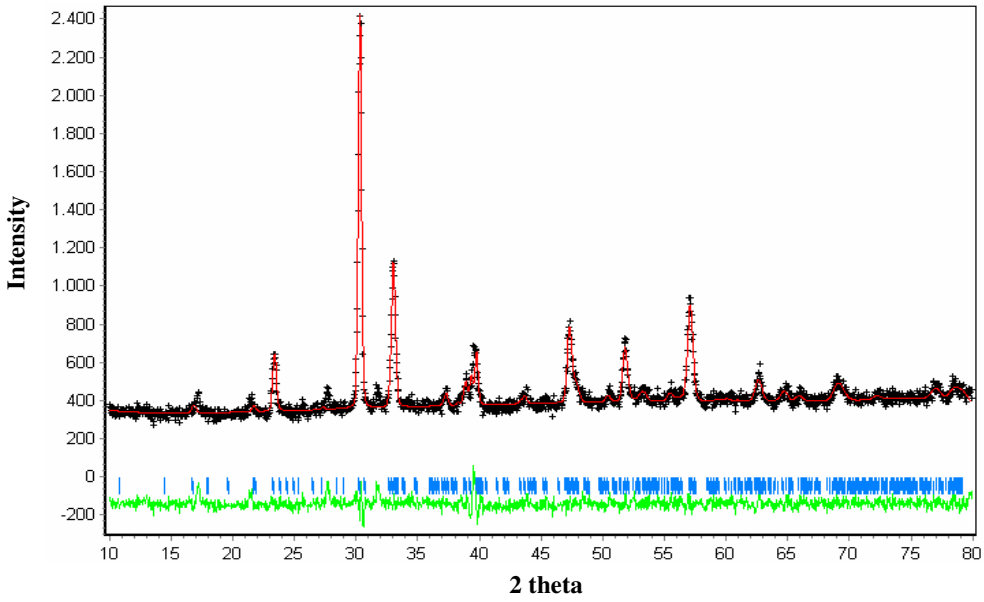
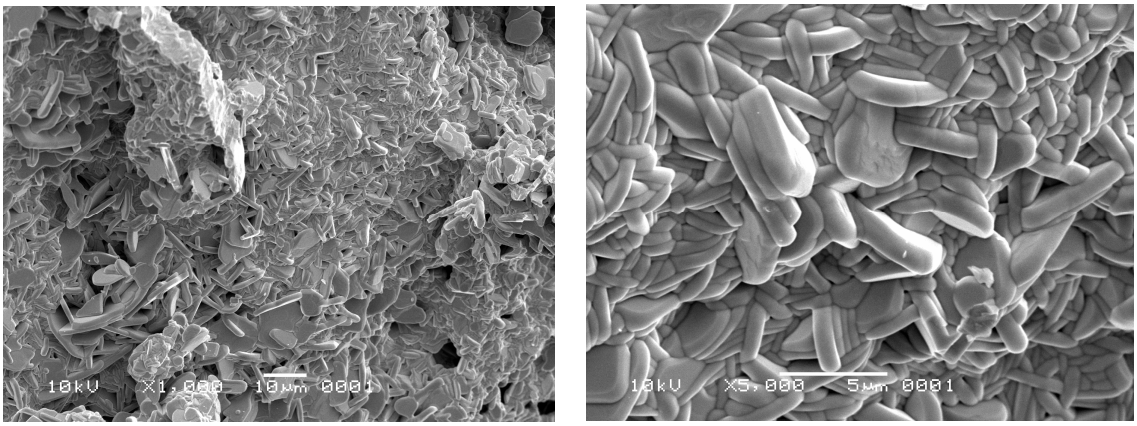


Figure 1 The Le Bail refinement plot showing the observed (+), calculated (red line), and their difference for BBT. This plot showed in space group *A21am* at room temperature.



(a) (b)

Figure 2 BBT with dilation, (a) 1000 x and (b) 5000x

Table 2 Comparation of composition using EDAX

Element	Massa (%)	Uncertainty (%)	Ar (gram/mol)	Mol comparation	Empiris formula
Ba	8.52	1.72	137.34	0.0820	1
Bi	68.85	0.78	208.98	0.3295	4

The SEM-EDAX is used to find information about surface morphology and element composition of BBT crystal. The morphology of BBT are non homogenous. The non homogenous crystal is predicted as a result of in complete reaction due to grinding. The crystal is predicted to be polycrystalline in Figure 2. Qualitative analyses using EDAX showed that Ba:Bi ratio in the crystal is 1:4 (Table 2).

Conclusions

The results are in excellent agreement with the data that reported in PDF (Powder Diffraction File) data base No. 84-1750 (orthorhombic). Particel size from BBT is calculated with Scherrer equation with the size of 219.967 Å. The surface analysis of $BaBi_4Ti_4O_{15}$ using SEM showed that the crystals are polycrystalline. Qualitative analyses using EDAX showed that Ba:Bi ratio in the crystal is 1:4.

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