

## Structural, Microstructural and Optical Studies of (Bi<sub>0.5</sub>Na<sub>0.5</sub>)TiO<sub>3</sub>-GdFeO<sub>3</sub> Solid Solution

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**Abstract.** The polycrystalline samples of ((Bi<sub>0.5</sub>Na<sub>0.5</sub>)<sub>1-x</sub>Gd<sub>x</sub>)(Ti<sub>1-x</sub>Fe<sub>x</sub>)O<sub>3</sub> (BNTGFO) with x=0.0 and 0.5 solid solution were prepared using a solid-state reaction technique. The formation of the desired materials and their structural properties were carried out by using the X-ray diffractions. Scanning electron microscope confirms the polycrystalline nature of the samples contains uniform grain distribution of unequal size. The presence of functional group was confirmed by Fourier transform infrared spectroscopy (FTIR).

**Keywords:** X-ray diffraction; SEM; FTIR.

### 1. Introduction

Ferroelectric perovskites are unique potential materials, which are widely used in commercial applications such as non-volatile ferroelectric memory, dynamic random access memory (DRAM), sensors and actuators [1]. Perovskite structure of (A<sub>0.5</sub><sup>3+</sup>A<sub>0.5</sub><sup>+</sup>TiO<sub>3</sub>) with two different cations at the A-site of the ABO<sub>3</sub> perovskite structure has been the recent interest of research. Particularly, bismuth sodium titanate Bi<sub>0.5</sub>Na<sub>0.5</sub>TiO<sub>3</sub> (BNT) compound until now has been a promising alternative to lead free piezoelectric ceramics [2]. Since, most of the ferroelectric materials used for application are Pb based, such as lead titanate (PbTiO<sub>3</sub>), lead zirconate titanate (Pb(Zr<sub>x</sub>Ti<sub>1-x</sub>)O<sub>3</sub>), lead lanthanum titanate (Pb<sub>1-x</sub>La<sub>x</sub>(Zr<sub>y</sub>Ti<sub>1-y</sub>)<sub>1-x/4</sub>O<sub>3</sub>) and lead magnesium titanate—lead titanate (Pb(Mg<sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub>—PbTiO<sub>3</sub> etc., [3]. In these ferroelectrics (FE), the Pb<sup>2+</sup> ions element is responsible for their intriguing properties, due to the lone pair electron; similar electronic configuration was found in Bi<sup>3+</sup> ions element and thus the scientific community is deep interested on BNT ferroelectric ceramics. The doping rare earth ions in Bi<sub>0.5</sub>Na<sub>0.5</sub>TiO<sub>3</sub> enhance its electrical as well as optical properties[4].The

advantage of rare earth doped BNT ceramics is that a large number of luminescent material for a wide range of application can be produced by using an optically active rare earth materials like  $\text{Eu}^{3+}$ ,  $\text{Pr}^{3+}$ ,  $\text{Sm}^{3+}$ ,  $\text{Nd}^{3+}$  ions these rare earth doped FE ceramics were used to develop multifunctional material for modern technology.

As no work on the composites/ system of BNT with rare earth orthoferrites was found in the literatures, we have planned to investigate the structural, micro structural and optical properties of the BNT-GdFeO<sub>3</sub> system of different ratios. All the rare earth orthoferrite family having the perovskite structure of general formula RFeO<sub>3</sub> (where R= rare-earth; La, Pr, Nd, Sm, Eu, Gd etc) display significant catalytic properties making these materials of great importance to be used in advance technologies as soft oxide fuels cells, catalysts, chemical sensors [5] and oxygen permeation membranes. Orthorhombic GdFeO<sub>3</sub> (GFO) has attracted considerable attention in recent years because its magnetic structure is similar to that in the well-known BiFeO<sub>3</sub> material. GdFeO<sub>3</sub> (GFO) is a well known ABO<sub>3</sub> perovskite oxide material which consists of FeO<sub>6</sub> octahedral units with Gd<sup>3+</sup> ions inserted between these units. GFO at room temperature has orthorhombic unit cell with Pbnm space group. It contains only trivalent iron and exhibits a high value of the Neel temperature ( $T_N$  -678<sup>0</sup>K) and ferroelectric transition at 700<sup>0</sup>K. It has also been reported that GFO demonstrate the multiferroic property and the polarization and magnetic coupling through magneto-capacitance measurement as a function of magnetic field. [6]. In this present work we have studied the structural, microstructural and optical properties of (((Bi<sub>0.5</sub>Na<sub>0.5</sub>)<sub>1-x</sub>Gd<sub>x</sub>)(Ti<sub>1-x</sub>Fe<sub>x</sub>)O<sub>3</sub>) (BNTGFO) with x=0.0 and 0.5 solid solution.

## **2. Experimental:**

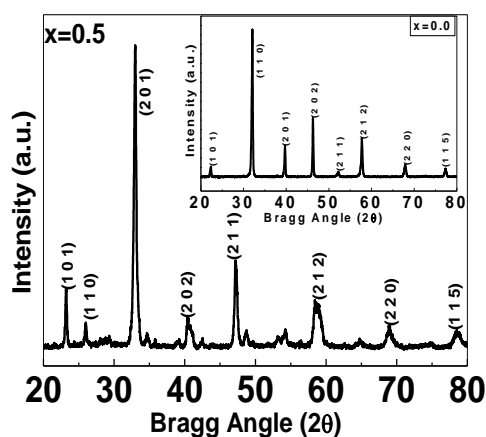
Polycrystalline samples of (((Bi<sub>0.5</sub>Na<sub>0.5</sub>)<sub>1-x</sub>Gd<sub>x</sub>)(Ti<sub>1-x</sub>Fe<sub>x</sub>)O<sub>3</sub>) (BNTGFO) with x=0.0 and 0.5 were prepared using AR grade ( $\geq 99\%$ ) precursors: Bi<sub>2</sub>O<sub>3</sub>, Na<sub>2</sub>CO<sub>3</sub>, TiO<sub>2</sub>, Na<sub>2</sub>CO<sub>3</sub>, Fe<sub>2</sub>O<sub>3</sub> & Gd<sub>2</sub>O<sub>3</sub> using a standard solid-state reaction (mixed oxide) technique. The homogeneous mixtures were calcined within a range of temperatures from 800<sup>0</sup>C to 900<sup>0</sup>C 4 h. The pellets (10 mm diameter and 1–2 mm thickness) of the above systems were prepared using a hydraulic press at  $5 \times 10^6$  N-m<sup>-2</sup>, which were sintered within a range of temperatures from 850<sup>0</sup>C-950<sup>0</sup>C. The X-ray diffraction patterns of the sintered pellets were recorded at room temperature with CuK <sub>$\alpha$</sub>  radiation ( $\lambda=1.5405\text{\AA}$ ) in a wide range of Bragg angle ( $20^0 \leq 2\theta \leq 80^0$ ) at a scan speed of 3<sup>0</sup>/min. The FTIR spectrums of the

specimens were measured by spectrometer using KBr method for the wave number range of  $500\text{-}4500\text{cm}^{-1}$ .

### 3. Result and discussion

#### 3.1. Structural and micro structural properties

Figure 1 shows the XRD patterns of BNTGFO. The distinct and sharp diffraction pattern of BNTGFO solid solution was suggesting the formation of single-phase new system. All the peaks of the XRD pattern of the samples were indexed in the hexagonal unit cell. A hexagonal unit cell was selected on the basis of good agreement between observed and calculated inter planar spacing for further structural analysis. The indexing of planes and refinement of the selected cell parameters were carried out using standard computer software (POWDD) [7]. It indicates that for different doping concentration of  $\text{GdFeO}_3$  in BNT in BNTGFO system can be used to form a single-phase perovskite (i.e., hexagonal) structure with good crystallization. The calculated cell parameters are  $a=5.5133\text{\AA}$ ,  $c=6.8437\text{\AA}$ ,  $V=180.15\text{\AA}^3$ .



**Fig. 1.** XRD pattern of (BNTGFO)  $x=0.0$

Figure 2 shows the surface microstructures or textures of  $((\text{Bi}_{0.5}\text{Na}_{0.5})_{1-x}\text{Gd}_x)(\text{Ti}_{1-x}\text{Fe}_x)\text{O}_3$  (BNTGFO) with  $x=0.0$  and  $0.5$  solid solution. The micro structural properties of the samples were studied by Scanning Electron Microscope. It confirms the polycrystalline nature of the samples contains uniform grain distribution of unequal size. All the sample surface grains present irregular geometry with compact structure [8].

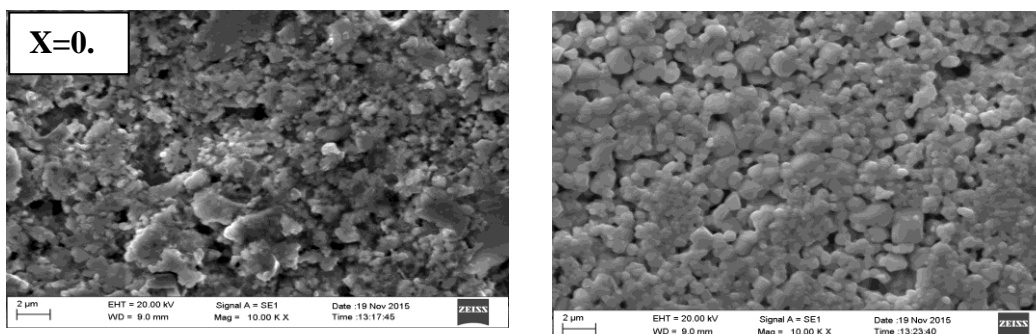
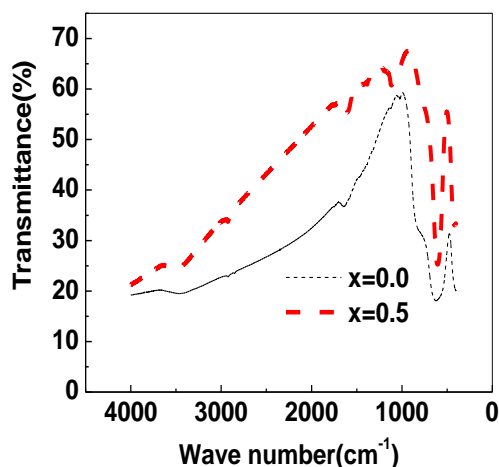


Fig. 2. SEM micrograph of (BNTGFO)

### 3.2 Optical Properties

#### 3.2.1 IR spectroscopic analysis

The FTIR spectra of  $((\text{Bi}_{0.5}\text{Na}_{0.5})_{1-x}\text{Gd}_x)(\text{Ti}_{1-x}\text{Fe}_x)\text{O}_3$  (BNTGFO) with  $x=0.0$  and  $0.5$  solid solution are shown in Figure 3. The FT-IR spectrum shows two strong absorptive bands at about  $560\text{cm}^{-1}$  and  $400\text{cm}^{-1}$  which correspond to Fe–O stretching vibration and O–Fe–O bending vibration of perovskite  $\text{GdFeO}_3$ , respectively. As well as it assign to the Ti–O stretching of octahedral groups in the perovskite structure. The bands between  $610$  and  $670\text{cm}^{-1}$  were the water libration (hindered rotation). This finding proves the formation of the perovskite  $\text{GdFeO}_3$  and is in accordance with the XRD data. Also, in the FT-IR spectrum of  $\text{GdFeO}_3$  nano powder weak bands were observed in the  $1300\text{--}1500\text{cm}^{-1}$  regions which are attributable to carbonate groups [9]. It is concluded that the carbonates the perovskite-type  $\text{GdFeO}_3$  by IR are formed mainly on the surface due to exposure to ambient air. The surface of the  $\text{GdFeO}_3$  particles obtained from the decomposition of the hetero-nuclear compound is more active to chemisorptions of gases such as  $\text{CO}_2$  in ambient, leading to the formation of carbonate ions. The asymmetric bands are assigned to the stretching vibration of octahedral  $\text{BO}_6$  groups in perovskite structure and confirming B–O bonds.



**Fig. 3** FTIR spectra of (BNTGFO).

The spectra shows prominent bands near  $3430\text{cm}^{-1}$  and  $1640\text{cm}^{-1}$  which are attributed to the stretching modes [10].

#### 4. Conclusion

The BNTGFO ceramic has been prepared by a high-temperature solid-state reaction technique. Preliminary X-ray analysis confirms the single phase crystal structure at room temperature. Scanning Electron Microscope confirms the polycrystalline nature of the samples contains uniform grain distribution of unequal size. All the sample surface grains present irregular geometry with compact structure. The presence of functional group was confirmed by Fourier transform infrared spectroscopy (FTIR).

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