

Structural and Optical Studies of $(\text{Sm}_x\text{Bi}_{0.5-x}\text{Na}_{0.5}\text{TiO}_3)_y\text{-(BiFeO}_3)_{1-y}$ Solid Solution

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Abstract. $(\text{Sm}_x\text{Bi}_{0.5-x}\text{Na}_{0.5}\text{TiO}_3)_y\text{-(BiFeO}_3)_{1-y}$ multiferroic ceramics ($y=0.0$ and $x=0.03$ for $y=0.05$) were synthesized by solid state reaction method. Preliminary X-ray structural analysis shows that SBNT-BFO polycrystalline compounds have rhombohedral crystal structure. The effect of samarium doping on structure and microstructure and optical properties is systematically investigated.

Keywords: X-ray diffraction; SEM; FTIR

1. Introduction

Multiferroic materials, in which electric and magnetic ordering coexist in a single phase, have attracted a lot of attention. Indeed, the coupling between the corresponding order parameters opens interesting perspectives for the designing novel applications in fields of microelectronics and spintronics [1]. Among all known multiferroics, only BiFeO_3 possesses spontaneous polarization and magnetic ordering at room-temperature. Uniquely high transition temperatures (antiferromagnetic Neel and ferroelectric Curie temperatures are about 640 and 1100 K, respectively) make this compound one of the most popular objects of the modern materials science [2]. On the other hand, possibilities of practical applications. In recent years, the accurate characterisation of the electronic structure of BFO by Density Functional theory (DFT) remains elusive, although there have been a number of studies devoted to this [3,4]. Bismuth sodium titanate $\text{Bi}_{0.5}\text{Na}_{0.5}\text{TiO}_3$ (BNT) compound until now has been a promising alternative to lead free piezoelectric ceramics [5]. Since, most of the ferroelectric materials used for application are Pb based, such as lead titanate (PbTiO_3), lead zirconate titanate ($\text{Pb}(\text{Zr}_x\text{Ti}_{1-x})\text{O}_3$), lead lanthanum titanate ($\text{Pb}_{1-x}\text{La}_x(\text{Zr}_y\text{Ti}_{1-y})_{1-x/4}\text{O}_3$) and lead magnesium titanate – lead titanate ($\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$ – PbTiO_3 etc., [6].

In these ferroelectrics (FE), the Pb^{2+} ions element is responsible for their intriguing properties, due to the lone pair electron; similar electronic configuration was found in Bi^{3+} ions element and thus the scientific community is deep interested on BNT ferroelectric ceramics. The doping rare earth ions in $\text{Bi}_{0.5}\text{Na}_{0.5}\text{TiO}_3$ enhance its electrical as well as optical properties[7]. 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 Eu^{3+} , Pr^{3+} , Sm^{3+} , Nd^{3+} ions these rare earth doped FE ceramics were used to develop multifunctional material for modern technology. All the rare earth orthoferrite family having the perovskite structure of general formula RFeO_3 (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 [8-11].

In this present work along with parent BFO material we doped Samarium modified BNT in different composition and studied the morphology, structure and optical properties for various device applications.

2. Experimental

Polycrystalline samples of $(\text{Sm}_x\text{Bi}_{0.5-x}\text{Na}_{0.5}\text{TiO}_3)_y-(\text{BiFeO}_3)_{1-y}$ ($y=0.0$ and $x=0.03$ for $y=0.05$)(SBNTFO) were prepared using AR grade ($\geq 99\%$) precursors: Bi_2O_3 , Na_2CO_3 , TiO_2 , Sm_2O_3 and Fe_2O_3 using a standard solid-state reaction (mixed oxide) technique. The homogeneous mixtures were calcined within a range of temperatures from 800°C to 900°C for 4 hrs. The pellets (10 mm diameter and 1–2 mm thickness) of the above systems were prepared using a hydraulic press at $5 \times 10^6 \text{ N-m}^{-2}$, which were sintered within a range of temperatures from 850°C - 950°C . The X-ray diffraction patterns of the sintered pellets were recorded at room temperature with CuK_α radiation ($\lambda=1.5405\text{\AA}$) in a wide range of Bragg angle ($20^\circ \leq 2\theta \leq 80^\circ$) at a scan speed of $3^\circ/\text{min.}$ The micro structural studies of the samples were carried out using Scanning Electron Microscope (EVO 18, Carl Zeiss Microscopy Limited). The FTIR spectrums of the specimens were measured by spectrometer (PerkinElmer FT-IR spectrum-2 94546) using KBr method for the wave number range of $400\text{-}4500\text{Cm}^{-1}$.

3. Result and discussion

3.1. Structural and micro structural properties:

Figure 1 shows the XRD patterns of $(\text{Sm}_x\text{Bi}_{0.5-x}\text{Na}_{0.5}\text{TiO}_3)_y-(\text{BiFeO}_3)_{1-y}$ ($y=0.0$ and $x=0.03$ for $y=0.05$)(SBNTFO). The distinct and sharp diffraction

pattern of solid SBNTFO 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 (POWD) [12]. It indicates that for different doping concentration of SBNT in BFO In the system can be used to form a single-phase perovskite (i.e., hexagonal) structure with good crystallization. The calculated cell parameters are $a=5.590 \text{ \AA}$, $c=13.887 \text{ \AA}$, ($y=0.00$) and $a=4.5204 \text{ \AA}$, $c=16.0617 \text{ \AA}$ (For $x=0.03(y=0.05)$). Figure 2 shows the surface microstructures or textures of SBNTFO with $y=0.0$ and $x=0.03$ (for $y=0.05$) solid solution.

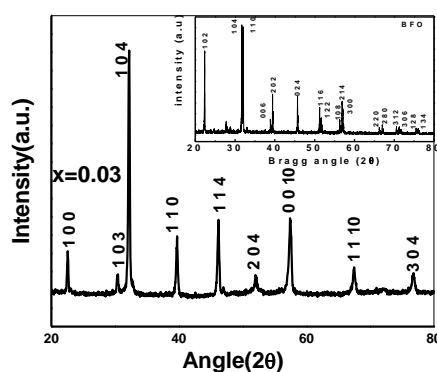


Figure 1. XRD pattern of $(\text{Sm}_x\text{Bi}_{0.5-x}\text{Na}_{0.5}\text{TiO}_3)_y-(\text{BiFeO}_3)_{1-y}$ For $x=0.03(y=0.05)$ BFO (insert).

Figure 2 shows the surface microstructures or textures of SBNTFO with $y=0.0$ and $x=0.03$ (for $y=0.05$) 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.

3.2 FTIR Spectroscopy

The IR spectrum also provides information about the chemical and molecular structural changes in BFO due to the changes in Fe-O bond during sintering as well as on doping with foreign atoms. The band between 700 cm^{-1} and 400 cm^{-1} is attributed to formation of metal oxides. The fundamental absorptions

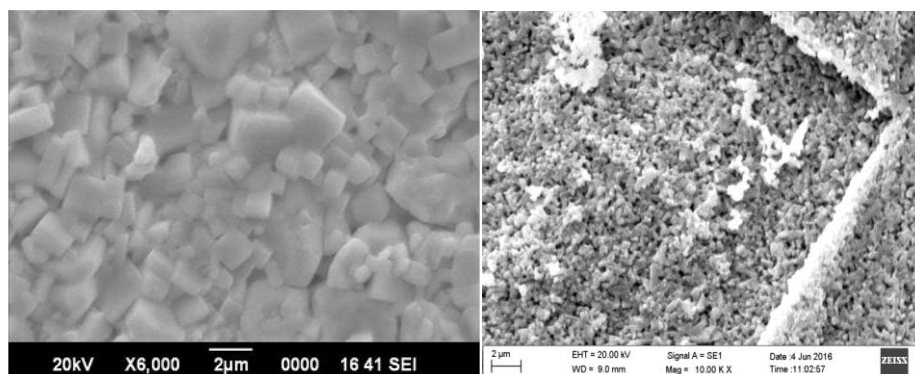


Figure 2. (a) SEM of $(\text{Sm}_x\text{Bi}_{0.5-x}\text{Na}_{0.5}\text{TiO}_3)_y-(\text{BiFeO}_3)_{1-y}$ for BFO ($y=0.0$) and, Fig. 2(b) For $x=0.03$ ($y=0.05$)

are observed in the wavelength region of 450 cm^{-1} to 550 cm^{-1} . This band is attributed to bending vibration of Fe-O bond in the FeO_6 octahedral unit and also to the BiO_6 octahedral structural unit. [13]. The BiO_6 octahedral structural unit also possesses vibrational modes between 600 cm^{-1} and 400 cm^{-1} . The very gradual shift in frequency of the Fe-O stretching mode indicates solid-solution formation. It indicates that substituent ions are at the corresponding sites in BFO.

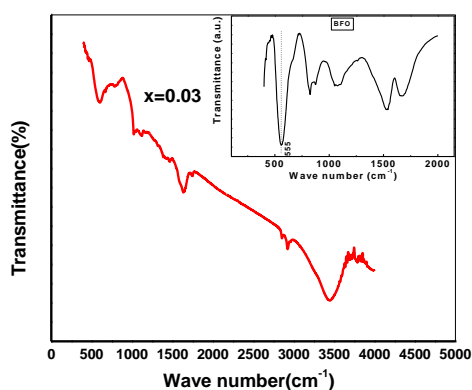


Figure 3. FTIR spectra of $(\text{Sm}_x\text{Bi}_{0.5-x}\text{Na}_{0.5}\text{TiO}_3)_y-(\text{BiFeO}_3)_{1-y}$ For $x=0.03$ BFO (insert).

4. Conclusion

The ceramic $(\text{Sm}_x\text{Bi}_{0.5-x}\text{Na}_{0.5}\text{TiO}_3)_y-(\text{BiFeO}_3)_{1-y}$ (SBNTFO) 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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