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Structural and Electrical Properties of $Bi(Fe_{0.8}La_{0.2})O_3$ Ceramic

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Abstract: La-modified $BiFeO_3$ perovskite ceramic i.e. $Bi(Fe_{0.8}La_{0.2})O_3$ is fabricated by a well-established solid-state reaction technique. The observed characteristics properties were analyzed by discrete characterization tools such as X-ray diffractometer (XRD) and scanning electron microscope (SEM). Thorough examinations of electrical properties of $Bi(Fe_{0.8}La_{0.2})O_3$ in an extensive frequency (10 kHz –500 kHz) and temperature (298K – 573K) ranges have presented a collection of interesting results concerning the structural and dielectric property relationship. The low tangent loss values of the prepared ceramic are useful for microwave applications.
Keywords: Fabricated, diffractometer, ceramic , structural.

1. Introduction

Ferroic materials which contains two or more than two ferroic orders simultaneously, are known as multiferroic material. From the time of its discovery, multiferroic materials have gathered massive consideration because of its extra degrees of freedom in device fabrication of electrical phenomenon devices and applications like random access memory, information storage media, spintronics and sensors, etc.[1]. $BiFeO_3$ i.e. BFO is one of the most studied multiferroic, among all available multiferroics. In BFO, the stereochemical activity of the Bi single electron pair contributes to ferroelectric polarization whereas the moderately filled 3d orbitals of the Fe^{3+} ions produce G-type antiferromagnetic order, which is clarified by its remarkably high transition temperatures (magnetic ordering occurs up to $T_N \approx 640$ K and ferroelectric ordering continues up to $T_C \approx 1100$ K). Such

features are exceptional, considering that most magnetic ferroelectrics exhibit simultaneous spin and dipole order only underneath room temperature. The crystal structure of BFO (polar phase) is represented within the *R3c* space group (rhombohedral)[2]. Kumar et al. observed that the modification of (La, Ti) in $BiFeO_3$ carries an inferior coactivity with small loss coefficient. It is well known that attempts were made to tailor the physical properties of bismuth ferrite by adding Rare-Earth and transition metal ions in the A-site or B-site of bismuth ferrite[3]. In La modified $BiFeO_3$ bulk ceramics, the improvement of ferroelectric properties might appear because of a decrease in secondary phases, oxygen vacancy and instability in valency of Fe that enlarges leakage current[4,5]. Morphological and electrical properties were examined by exploiting a scanning electron microscope (SEM) and N4L LCR meter (computer-controlled) respectively. Additionally, it will provide perception into the characteristics of relaxation of the examined compound. The dielectric, structural and elemental properties are examined in this research article.

2. Experimental Procedure

The ceramic compound exhibiting chemical compositional formula $Bi(Fe_{0.8}\ La_{0.2})O_3$ was synthesized by following the general solid state reaction method. High quality of analytical rating oxides such as; bismuth oxide (Bi_2O_3), lanthanum oxide (La_2O_3) and iron oxide (Fe_2O_3) were exploited as primary raw ingredients. High quality alumina crucibles (cylindrical), boats and trays were used in making of La-modified BFO ceramic compound. Distilled water was utilized for synthesizing the poly-vinyl alcohol solution. The starting materials of solid-state reaction method were carefully weighed in stoichiometry ratio followed by the methodically mixing with the use of mortar and pestle (dry medium), later in methanol (wet medium) for 6 hrs. The X-Ray Diffraction data collection was completed by using CuK_α (λ = 1.5405 Å) radiation, exploiting Rigaku (Ultima-IV) powder diffractometer stimulated at a slow scan speed (0.02 step in 2θ) over the angular range of Bragg angles ($20^0 \leq 2\theta \leq 80^0$). The obtained powder was grinded again and it was pressed into 12 mm diameter, 1.5 mm thickness pellets by using hydraulic press. Finally, the synthesized ceramic compound pellets were sintered at 1123 K for 5 hrs, which provides an increment in density of pressed pellets.

3. Result and discussion

Structure and Microstructure:The crystallographic studies of $Bi(Fe_{0.8}La_{0.2})O_3$ ceramic has been conducted by the use of X-ray diffractometer at room temperature, as shown in Figure 1. Inserting the XRD data in the 'POWDMULT' software, the preliminary crystalline property and structural analysis of as prepared $Bi(Fe_{0.8}La_{0.2})O_3$ sample was carried out. It is shown in the figure that most of the peaks have tall and thin intensities. These peaks suggest a decent as well as the crystalline characteristics of the synthesized compound.

Detected XRD reflection peaks were indexed and fulfilled the required properties of perovskite structure of the orthorhombic symmetry with good agreement. The POWDMULT software uses least-square method to obtain the lattice parameters. The refined lattice parameters of the synthesized compound were acquired as, $a = 4.2614$ Å, $b = 10.7866$ Å, $c = 35.4891$ Å with the lowest value of standard deviation (SD= 0.0027 Å). To determine the crystallite size (D), XRD data is substituted in the Scherrer formula. By substituting the broadening of reflection peak (β), position at Bragg angle (2θ) and the wavelength (λ) in the following Scherrer formulism, D is calculated.

$$D = \frac{k\lambda}{\beta \cos\theta}, \tag{3.1}$$

where, $k = 0.89$ (Scherrer constant). The average crystallite size was obtained to be 31.42 nm. The structural constancy, defined as tolerance factor (T_F) of the ABO_3-like perovskite ceramic compound, is constructed on the following equation.

$$T_F = \frac{\left(\langle R_A \rangle + R_O\right)}{\sqrt{2}\left(\langle R_B \rangle + R_O\right)}. \tag{3.2}$$

Here $\langle R_A \rangle$, $\langle R_B \rangle$ & R_O signify average ionic radii of the A (bismuth), B (lanthanum & iron) and O (oxygen) site(s) respectively. The character T_F tells the structural dependability of the perovskite family. For $Bi(Fe_{0.8}La_{0.2})O_3$, the calculated value of tolerance factor is 0.76, which

suggests foremost deviation and distortion in mentioned perovskite structure of the material.

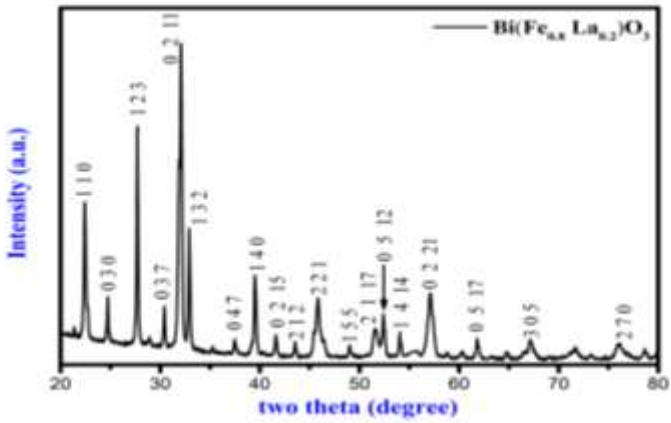

Figure 1. XRD of $Bi(Fe_{0.8}\ La_{0.2})O_3$

Figure 2(A) demonstrates the SEM image of the synthesized ceramic compound. The surface architecture advises good and high density of grains with a continuous surface. The dense grain progress is because of the sintering of the synthesized compound at higher temperature. Figure 2(B) displays the EDS, signifying that the occurrence of essential elements like Bi, La, Fe, O without any hints of impurity taking place in the synthesized compound.

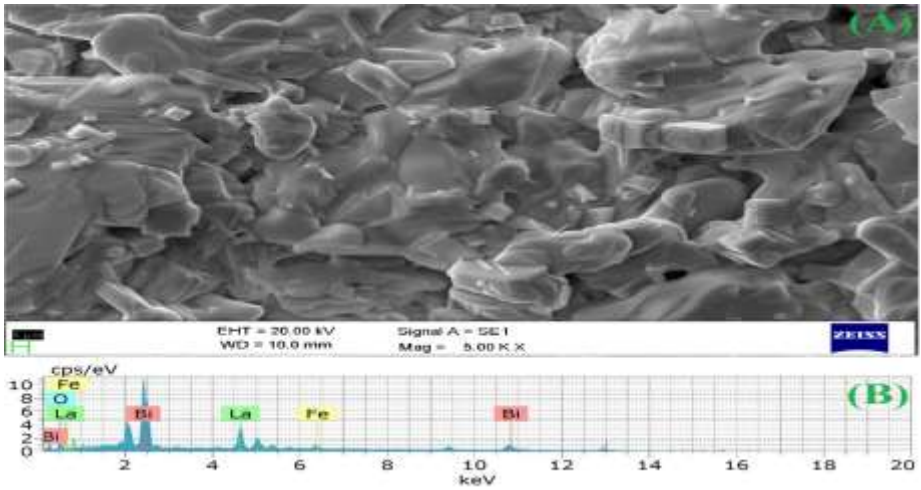

Figure 2. SEM and EDS of $Bi(Fe_{0.8}\ La_{0.2})O_3$

4. Dielectric Study

The dielectric analysis is one of the important and significant method for synthesized ceramic compounds. It provides the data concerning both the dielectric parameters i.e. dielectric constant (ε_r) and dielectric loss $(\tan\delta)$ of a specimen ceramic compound under the fixed direction of electric field and operational frequency depend on the types of polarization, which is responsible for the relaxation mechanism in a material. Both the dielectric parameters were evaluated by the exploitation of phase-sensitive multimeter, associated mutually with the temperature-controlled furnace and computer. Both dielectric parameters (ε_r) and $(\tan\delta)$ of the synthesized compound were calculated by the universal capacitance measurements at selected frequencies as well as temperatures[6,7].

$$\varepsilon = \frac{d}{\varepsilon_0 A} C_{11} \ . \tag{4.1}$$

Here $\varepsilon =$ Dielectric constant, $C_{11} =$ parallel capacitance (experimentally), $d =$ thickness of pellet, $\varepsilon_0 =$ free space permittivity and $A =$ area of pellet

Figure 3 (a-b) demonstrate the dissimilarity among dielectric constant (ε_r) and tangent loss $(\tan\delta)$ of the synthesized ceramic compound. We observed that the outcome demonstrated both dielectric parameters values rises and moderately declines with the increase in temperature at all operating frequencies. However, the result of both ε_r and $\tan\delta$ decreases with an increasing the functioning frequency, which is because of the universal characteristic of dielectrics. For lower frequency, all type of polarization (dipole, ionic, interfacial and atomic) happen in dielectrics. This kind of polarization nature regularly vanishes with an increase in frequencies. Subsequently, the dielectric constant outcome decreases. The dielectric plots display as-synthesized ceramic compound owns temperature-dependent dielectric constant. The increasing trend in the dielectric constant outcome of the material is a little increasing in the lower temperature range (298 K to 323 K), but above operational temperature range (323 K to 473 K), the dielectric constant parameters quickly upsurge for all selected frequencies. The variation of the growing trend in tan δ value at the low-temperature section (from 298K to 370 K) is marginal, further at high temperature range (370 K up to 573 K), the dielectric trend quickly increases for all nominated frequencies.

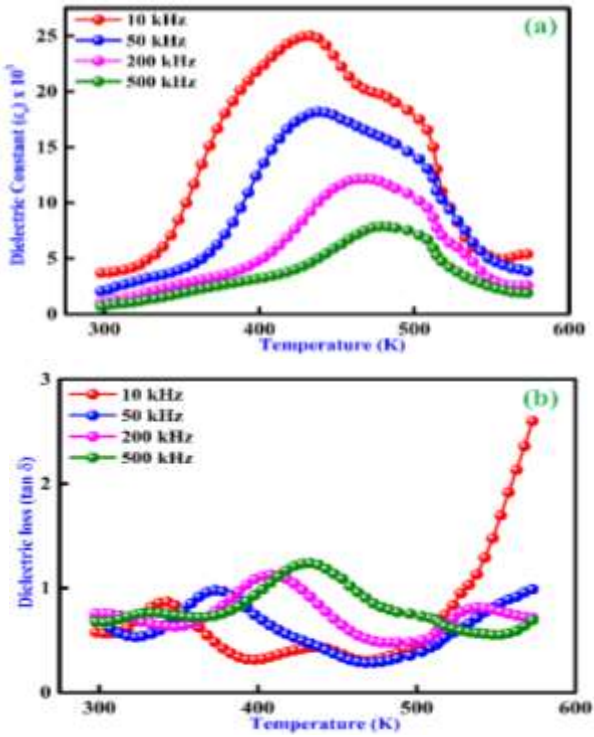

Figure 3. Temperature Dependent dielectric constant plots for $Bi(Fe_{0.8}\ La_{0.2})O_3$

As an outcome, the electron-phonon interaction might be the cause for growing dielectric constant value with a growth in temperature[8]. Furthermore, thermally activate scattering of charge carriers and the existence of oxygen vacancies might be the reason for a shrill increase in the tanδ outcome at higher temperatures for the $Bi(Fe_{0.8}\ La_{0.2})O_3$ material. The calculated outcomes of temperature-dependent dielectric constants are given in the table 1.

Table 1 Temperature dependent ε_r tanδ values of $Bi(Fe_{0.8}\ La_{0.2})O_3$

S. No	Frequency	Temperature 298 K		Temperature 573 K	
		Dielectric Permittivity ($x10^3$)	Dielectric Loss	Dielectric Permittivity($x10^3$)	Dielectric Loss
1	10 kHz	3.7012	0.576	5.3733	2.599
2	50 kHz	2.0517	0.724	3.8262	0.987
3	200 kHz	1.0533	0.754	2.5793	0.714
4	500 kHz	0.6898	0.677	1.8780	0.691

5. Conclusion

Present research work demonstrates XRD study of Polycrystalline $Bi(Fe_{0.8}\ La_{0.2})O_3$ ceramic compound presented an orthorhombic crystal system. The mean D (i.e. average crystallite size) of the synthesized ceramic compound was calculated approximately 31.42 nm (estimated from the broadening of reflection peaks by using Scherrer's formula), varying between 49.45 nm to 11.40 nm. The SEM surface architecture displays the consistent and uniform grain-distribution of different dimensions. Both dielectric parameters (ε_r and $\tan\delta$) are very much influenced by the temperature and frequency of the applied ac electric field. As an outcome of the low tangent loss, the quality factor (Q factor) of the synthesized ceramic compound is very large and this is a standard for numerous applications like microwave laminates and appliances.

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