

Structural and Electrical Characteristics of $\text{Bi}(\text{Fe}_{0.95}\text{Y}_{0.05})\text{O}_3$ Ceramic

Alok Shukla and L. Thansanga

Department of Physics
National Institute of Technology Mizoram, Aizawl-796012, India
Email: aloks.nitmz@gmail.com

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Abstract: In this work, studies of the structural and electrical characteristics of yttrium (Y) substituted bismuth ferrite (BiFeO_3) at Fe-site with a composition of $\text{Bi}(\text{Fe}_{0.95}\text{Y}_{0.05})\text{O}_3$ (abbreviated as BFYO5) has been reported. BFYO5 material has been synthesized through a conventional solid state reaction method. The basic crystal data and phase formation were analyzed by using X-ray diffraction (XRD). Detailed studies of the effect of Y (5%) substitution on electrical properties of BiFeO_3 has been examined by using phase sensitive multimeter (PSM) in a wide range of temperature (25-350⁰C) and frequency (1-1000 kHz), which provided a significant enhancement in the electrical properties of bismuth ferrite. Our results confirmed that yttrium doped BiFeO_3 at Fe-site is an effective way to rectify various issues relevant for device applications.

Keywords: Multiferroic, X-ray diffraction, Bismuth ferrite, Solid state reaction, Electrical characteristics.

1. Introduction

Recent years, the multiferroic material, which exhibits ferroelectric and ferromagnetic properties simultaneously in a single phase have greatly drawn an attentions of researchers because of their potential applications in various devices such as data storage media, multi-state memories, spintronic, microelectronic devices and transducers, etc.¹⁻⁴. Among few multiferroic materials, BiFeO_3 is one of the most studied compound as it has ferroelectric and anti-ferromagnetic ordering simultaneously at above the room temperature ($T_c = \sim 830^0\text{C}$ and $T_N = \sim 370^0\text{C}$)⁵. It has rhombohedrally-distorted perovskite crystal structure with R3c space group. The ferroelectric

property of BiFeO_3 occurs due to the existence of 6s lone pair electrons of Bi^{+3} ions while the anti-ferromagnetic order is due to Fe^{+3} ions⁶. Unfortunately, BiFeO_3 has some inherent problems such as high current leakage, high dielectric loss, structural distortion, etc., which restricts its practical applications in electronic devices as it effects the structure and the value of dielectric and electrical properties.

In order to overcome the above problems, much efforts have been paid by applying several doping at Bi/Fe-site of BiFeO_3 . A substitution of BiFeO_3 some rare earth and other elements had also been carried out in the last few decades^{7,8}. From the literature reviews, a significant enhancement in the multiferroic properties of BiFeO_3 has been observed by substituting divalent ion or trivalent ion at the Bi and Fe-site respectively^{9,10}. Therefore, in this work, a systematic study of the effect of yttrium substitution at Fe-site of BiFeO_3 has been reported.

2. Experimental

A polycrystalline sample of $\text{Bi}(\text{Fe}_{0.95}\text{Y}_{0.05})\text{O}_3$ was fabricated by using bismuth oxide (Bi_2O_3), iron oxide (Fe_2O_3) and yttrium oxide (Y_2O_3) through a solid state reaction method. All the ingredients were mixed thoroughly with the help of mortar and pestle in a dry air for 2 hrs and wet medium for another 2 hrs. The sample was calcined at 750°C for 6 hrs after homogeneously mixing. The calcined sample powder was then mixed with polyvinyl alcohol (as a binder), and make a disc shape pellet of 12 mm diameter by applying $4 \times 10^6 \text{ Nm}^{-2}$ by using a KBr hydraulic press. The disc shape pellet sample was then sintered at an optimised temperature 800°C for 6 hrs in air atmosphere. Finally, the sintered sample was polished by using a fine emery paper and electroded with a high quality silver paste for electrical measurements.

3. Results and Discussion

3.1 Structural analysis: Fig. 1 shows the room temperature powder XRD pattern of $\text{Bi}(\text{Fe}_{0.95}\text{Y}_{0.05})\text{O}_3$ compound. The X-ray diffraction technique was utilized for checking the phase formation of the studied material. The XRD peaks were indexed with a standard software 'POWDMULT'. Based on the agreement between observed and calculated inter planar spacing d value, the crystal system of the material changes from rhombohedral to orthorhombic symmetry due to the effect of yttrium 5% substitution at Fe-site of bismuth ferrite. The lattice parameters are: $a=9.5490 \text{ \AA}$, $b=8.6769 \text{ \AA}$, $c=10.8778 \text{ \AA}$

and volume $V=901.30 \text{ \AA}^3$ with a minimum standard deviation, $SD=0.033 \text{ \AA}$. The average crystallite size of the material was calculated by using Sherrer's formula, $P_{hkl}=K\lambda/\beta_{1/2} \text{ Cos}\theta$ and found to be 39 nm. Where K =constant that depends on a crystallite size, $\lambda=1.5418 \text{ \AA}$, $\beta_{1/2}$ =peak width of reflection at half height and θ =Bragg's diffraction angle.

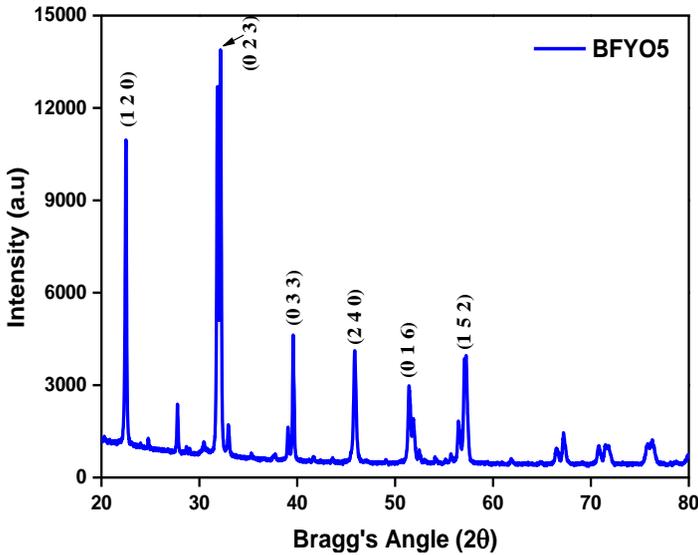


Figure 1. The X-ray diffraction pattern of Bi(Fe_{0.95}Y_{0.05})O₃ material in a diffraction angle 20⁰-80⁰.

3.2 Dielectric study: Fig. 2 shows the temperature dependence of dielectric constant (ϵ_r) and dielectric loss ($\tan\delta$) (inset image) at a wide range of frequency (1kHz-1MHz). The dielectric constant value of low frequency spectrum increases with the rise of temperature. Two peaks were observed at 150⁰C and 300⁰C due to the presence of antiferromagnetic transition¹¹. Whereas, a slow rate of increasing dielectric constant value throughout the temperature was observed in higher frequency spectra (500 kHz and 1 MHz) as compared with low frequency curve. The value of dielectric loss is almost constant up to 270⁰C for all the selected frequencies. However, a sharp increase of $\tan\delta$ occurs at 340⁰C as a result of thermally activated charge carriers and existence of small imperfections during the synthesis process. Both the dielectric parameters were increased at higher temperature and low frequencies probably due to interfacial polarization dominating over dipole polarization. On the other hand, dielectric constant and dielectric loss were decrease with increasing frequency, it is a general feature of dielectric materials. Different types of polarizations such as electronic, ionic, interfacial, atomic, dipole, etc. were exist in dielectric materials. All these

polarizations were gradually vanish with increasing frequency, and that subsequently results a decrease in dielectric constant.

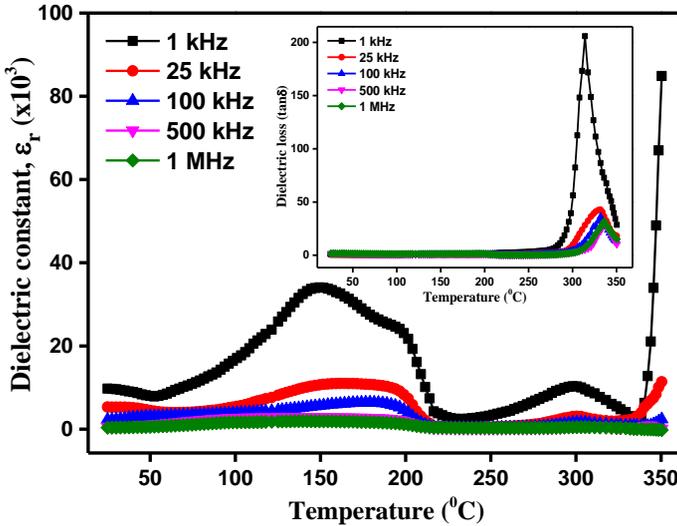


Figure 2. The variation of dielectric constant (ϵ_r) and dielectric loss ($\tan\delta$) (inset image) with temperatures at frequency (1kHz-1MHz) for $\text{Bi}(\text{Fe}_{0.95}\text{Y}_{0.05})\text{O}_3$ compound.

Fig. 3 shows the variation of frequency dependent dielectric constant and dielectric loss of $\text{Bi}(\text{Fe}_{0.95}\text{Y}_{0.05})\text{O}_3$ compound at a selected temperatures (25°C - 350°C). It has been observed from the plot that the value of dielectric constant is high at low frequency region, which gradually decreases with the rise in frequency, which is due to the fact that only a few dipoles followed the applied electric field at higher frequency region. So, the dielectric constant shows a dispersive spectrum at low frequencies. A decreasing trend of dielectric loss ($\tan\delta$) with increasing frequency is also observed at selected higher temperatures (300°C and 350°C) which probably due to the presence of iron in the compound¹². Whereas a small change in the value of $\tan\delta$ has been observed for lower temperature curves. At higher frequencies, both the dielectric parameters (ϵ_r and $\tan\delta$) remains almost constant at all the selected temperatures. This nature clearly indicates the presence of polar dielectrics in $\text{Bi}(\text{Fe}_{0.95}\text{Y}_{0.05})\text{O}_3$ compound.

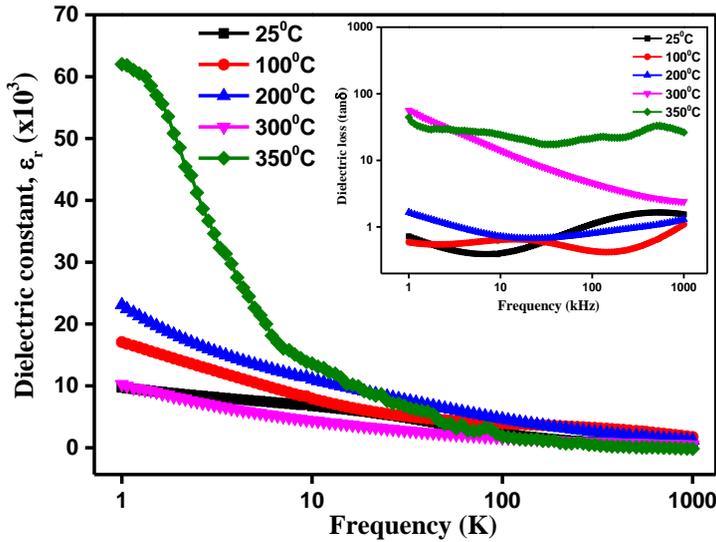


Figure 3. The variation of dielectric constant (ϵ_r) and dielectric loss ($\tan\delta$) (inset image) with frequency at selected temperatures (25°C , 100°C , 200°C , 300°C , 350°C) for $\text{Bi}(\text{Fe}_{0.95}\text{Y}_{0.05})\text{O}_3$ compound.

3.3 Impedance study: Fig. 4 shows the variation of a frequency dependent impedance (Z') of $\text{Bi}(\text{Fe}_{0.95}\text{Y}_{0.05})\text{O}_3$ at selected temperatures 25°C , 100°C , 200°C , 300°C and 350°C . The value of impedance (Z') gradually decreases with increase in temperature at the low frequency region, which clearly suggests the behavior of negative temperature coefficient of resistance of BFYO5 compound. At higher frequency region (40kHz-1MHz), all the curves of Z' were tend to merge to get nearly a constant value, which may be due to the release of space charge at this region¹³.

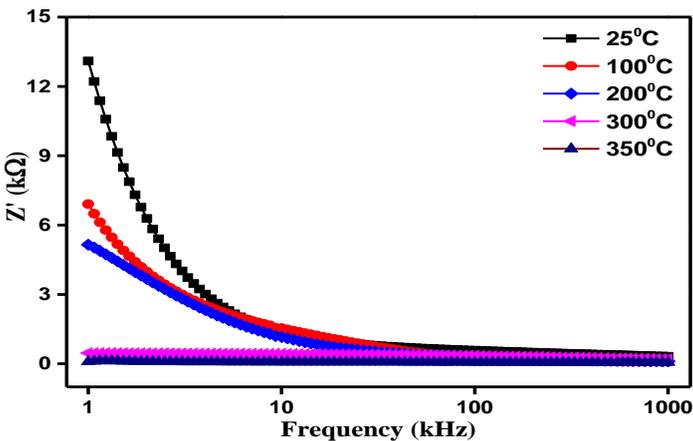


Figure 4. Variation of a frequency dependence of impedance (Z') at selected temperatures (25°C - 350°C)

3.4 AC-conductivity study: Fig. 5 represents the variation of ac-conductivity in a wide range of frequency (1-1000 kHz) at selected temperatures (25⁰C -350⁰C) for BFYO5 compound. The nature of ac-conductivity shows that the conductivity increases with the rise of frequency and temperature. The conductivity plot gradually rises and tend to merge at higher frequency region. A frequency independent nature has been observed in some of the selected temperature curves i.e. 300⁰C and 350⁰C. A suitable approach called ‘Jonscher’s power law’¹⁴ has been used for investigating the frequency dependent conductivity characteristics of the material as given below:

$$(3.1) \quad \sigma_{ac}(\omega) = \sigma_x + \sigma_y(\omega)$$

$$(3.2) \quad \sigma_{ac}(\omega) = \sigma_x + P\omega^\gamma$$

Where σ_{ac} = total conductivity, σ_x = frequency independent part, P and γ suggests range of interaction among the mobile ions with a crystallographic lattice sites and strength of polarizability respectively.

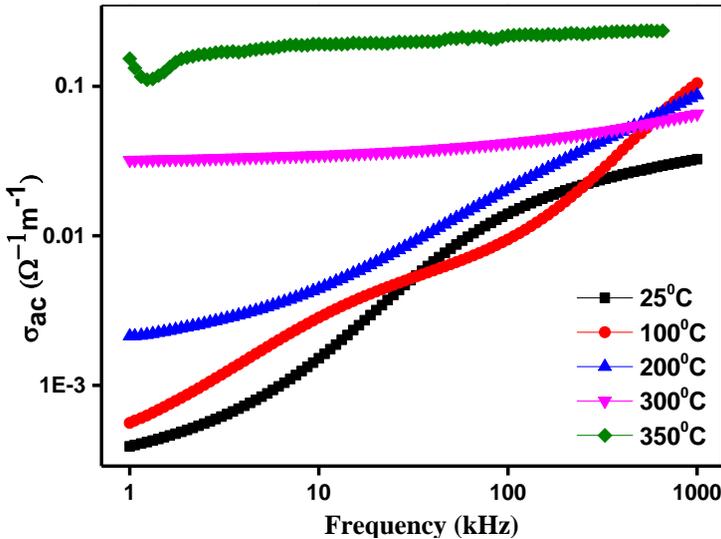


Figure 5. Variation of a frequency dependence of ac-conductivity σ_{ac} at selected temperatures (25⁰C -350⁰C) for Bi(Fe_{0.95}Y_{0.05})O₃ compound.

4. Conclusion

A single phase Bi(Fe_{0.95}Y_{0.05})O₃ compound has been successfully synthesized through a conventional solid state reaction method. The basic crystal data and phase formation were confirmed by using X-ray diffraction. The crystal system changes from rhombohedral to orthorhombic structure due to the effect of yttrium substitution. The average crystallite size of the compound was calculated using Scherrer's formula and found to be 39 nm. The dielectric constant and dielectric loss were highly dispersed at low frequency region and decreases with the rise of frequency and increases with increasing temperature. Study of conductivity of the compound shows negative temperature coefficient of resistance behavior. A significant enhancement in the electrical characteristics of BiFeO₃ has been observed from this work. Based on these significant enhancements, Bi(Fe_{0.95}Y_{0.05})O₃ could be considered as a promising candidate for advanced electronic devices.

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