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Synthesis and Structural Characterization of Ba Doped Bismuth Ferrite by Sol Gel Method for Cleaner Environment

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Abstract *–Barium doped bismuth ferrite samples with formula Bi_{1-x} Ba $_x$ FeO_3 (x=0.3, 0.4, 0.5) were synthesized by sol gel technique. The X –ray diffraction (XRD) studies confirmed the phase formation, phase purity of the synthesized samples. The enhancement in lattice parameters and hence the unit cell volume with increasing doping concentration is well in accordance with the Vegards's law. The increasing broadening of peaks with increasing doping concentration is attributed to the decrease in crystallite size. The enhancement in microstrain for increasing doping concentration(x=0.3, 0.4, 0.5) reported from the XRD studies also revealed that lattice gets more and more strained with increasing doping concentration.*

Keywords-Bismuth Ferrite, Ferroelectricity, XRD,sol-gel Antiferromagnetic,

I- INTRODUCTION

The multiferroics are the much sought after materials these days owing to their applications in versatile fields ranging from microwave devices, spintronics,sensors and energy devices [1, 2, 3,5,8]. The potential use of bismuth ferrite ($BiFeO_3$) in supercapacitors used for electric vehicles is well documented [6]. From the future perspective, bismuth ferrite is a highly promising material that can be used in the recycling of waste water and thereby controlling the pollution. The potential use of $BiFeO_3$ in pollution control, clean energy could prove to be a game changer keeping in view the ever increasing global demand for a cleaner environment and clean energy.

Bismuth ferrite is probably the only single phase multiferroic material which exhibits simultaneous ferroelectricity and antiferromagnetism at room temperature. Its relatively higher ferroelectric Curie temperature, T_C =1103K and antiferromagnetic Neel temperature ,T_N =643K makes it suitable for wide variety of applications[1,2,5,7,8].Not only its variety of technological applications but also the interesting fundamental science behind it makes the study of bismuth ferrite a rather fascinating and imperative one. It has rhombohedrally distorted perovskite structure with R3c space group [1,2,3,4,7,8].

Bismuth is highly volatile owing to the presence of lone pair of electrons. The high volatility of bismuth leads to problems of non-stoichiometry and impurities. Also the problem of oxygen vacancies result in high leakage current [1,4,5]. This along with the cycloidal spin structure makes it very much impossible to use it in its pure form. The problem can be overcome by synthesizing nanostructured materials [1,5]. The spin cycloid will be broken by synthesizing nanoparticles of the size comparable to that of spin cycloid which in turn

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leads to the improvement in the net magnetization of the material [1]. To add to this, doping bismuth ferrite with alkaline earth or rare earth element increases the resistivity of the material thereby eradicating the problem of high leakage current [2]. In the quest of overcoming these drawbacks and thereby realizing the tremendous applications of bismuth ferrite, we have doped it with alkaline earth element barium (Ba).The sol-gel method was employed for the synthesis of Ba doped bismuth ferrite samples. Here we intend to do the structural analysis of the samples using X-ray diffraction (XRD).

II -LITERATURE REVIEW

Chaudhary and Mandal reported decerase in crystallite size leading to distortion with increasing doping concentration of barium. The FESEM analysis of the samples confirmed the change in morphology of the samples [1].M.M. El-Desoky et al reported that the structure of Ba doped bismuth ferrite is rhombohedral-hexagonal one. Also the simultaneous existence of ferromagnetic and ferroelectric hysteresis loops in the samples at room temperature supports its candidature for use in spintronic devices and information storage [2].T. Durga Rao et al reported that the phase of $BiFeO_3$changed slightly from rhombohedral to orthorhombic on doping with rare earth elements like Yttrium, Holonium.The magnetization studies revealed that the obvious M-H loop observed in doped samples could be the result of breaking of spin cycloid and explained on the basis of weak ferromagnetism [3].Astita Dubey et al reported decrease in crystallite size, broadening of peaks on doping $BiFeO_3$ with Ba.The surface strain reported in the doped sample was due to the change in the magnetic properties [4].Mahendra Shisode et al reported the structural change from rhombohedral to hexagonal when barium is increasingly doped into $BiFeO_3$.The significant improvement in the magnetic and ferroelectric properties of the doped samples can be pivotal in applications like spintronics,data storage [5].Vijaykumar Jadhav reported the use of bismuth ferrite as potential candidate for use in supercapacitors which will be the core component of electric vehicles in future [6].Mostafavi et al inferred that there can be ienhancement in the multiferroic properties of $BiFeO_3$ on being doped with an ion having greater ionic radius.[7].

III - METHODOLOGY

Ba doped bismuth ferrite samples with formula Bi_{1-x} Ba $_x$ FeO_3 (x=0.3, 0.4, 0.5) were synthesized by sol gel technique..The sol gel method adapted for the synthesis is highly cost effective, requires lesser temperature, is less risky and does not require any sophisticated equipment.

All the chemicals used were from SD Fine Chemicals and were of AR grade having 99.99% purity. All the glasswares were washed with deionised water and then acetone so as to remove the impurities. The precursors bismuth nitrate [Bi $(NO_3)_3$, 5H $_2$O], Iron nitrate [Fe $(NO_3)_3$, 9H $_2$O] ,barium nitrate [$BaNO_3)_2$] were weighed in stoichiometric proportions. Citric acid acting as a chelating agent was added to the mixture of metal nitrates in stoichiometric proportion. The solution of the mixture of these metal nitrates and citric acid taken in the proportion 1:1 was prepared in 50 ml deionised water. The resulting solution was then stirred vigorously leading to a clear transparent solution. The P^H of the solution was maintained at 3 using 30% liquid ammonia. The solution so obtained was then heated to 90^0C for about 3 hours on a hot plate.till gel is formed. Ethylene glycol was added to the solution at regular intervals during the heating so as to impart homogeneity to the mixture.The gel so formed was then subjected to calcination in oven at 200 ^{0} C for 12 hours so as to make it completely dry and to facilitate the removal of unwanted gases from the mixture. The gel was finely powdered using mortar pastel. The powder was then sintered in the muffle furnace at 700 ^{0} C for 2 hrs so as to eliminate any remaining moisture if any and to facilitate phase formation.

IV- RESULT & DISCUSSION

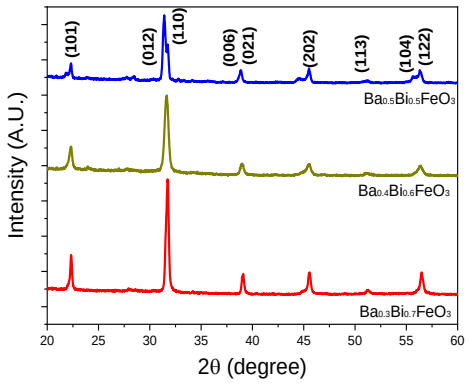

Fig1- X ray diffractograms for Bi_{1-x} Ba $_x$ FeO_3 (x=0.3, 0.4, 0.5)

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The X- ray diffraction patterns of the samples are as shown in Fig1.. X-ray diffraction was performed using a PAnalytical X-ray diffractometer with high intensity Cu Kα radiation.All the observed peaks for x=0.3,0.4 ,0.5 confirmed the phase formation of $BiFeO_3$ which has a rhombohedrally distorted perovskite structure with R3c space group.The structure of $BiFeO_3$ on doping with Ba gets transformed from rhombohedral to hexagonal [2,5].The indexing was done by ICSD reference pattern 417304 [4].The values of the ,lattice parameters cell volume ,crystallite size and microstrain are as depicted in Table1.The shifting of maximum intensity peaks towards lower 2Θ values with increasing Ba doping concentration results in broadening of peaks [4,5]. This can be attributed to the decrease in crystallite size with increasing doping concentration.The interplanar spacing d (in A^0) for the planes was calculated using Bragg's law.

The crystallite size(D) was calculated using Debye-Sherrer formula: $D = 0.89\lambda/\beta Cos\theta$……(1)
The lattice parameters were calculated using the formula: $\frac{1}{d^2} = \frac{4}{3}\frac{h^2+k^2+hk}{a^2} + \frac{l^2}{c^2}$-----……(2)

The unit cell volume was calculated using the formula: $V = 0.866\, a^2 c$. …… (3)

The increase in lattice parameters with increasing doping concentration clearly indicates that the doping of Ba causes more and more distortion of the rhombohedral perovskite structure of $BiFeO_3$. This significant increase in the lattice parameters and hence unit cell volume can be attributed to the greater ionic radius of Ba^{2+} (1.42 A^0) than Bi^{3+}(1.17 A^0) [7] .The Fig 2 shows the increase in lattice parameter with doping concentration.

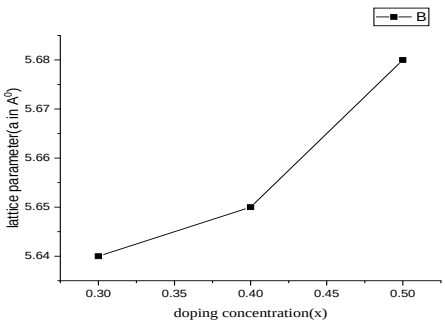

Fig 2 - Variation of lattice parameter with doping concentration

The increase in microstrain with increasing doping concentration confirms the increasing distortion of the crystal. The Fig 3 shows the variation of microstrain with doping concentration.

The decrease in crystallite size and increase in microstrain with increasing doping concentration makes it distinctly evident that there is more and more incorporation of Ba^{2+}at the Bi^{3+} site of $BiFeO_3$.

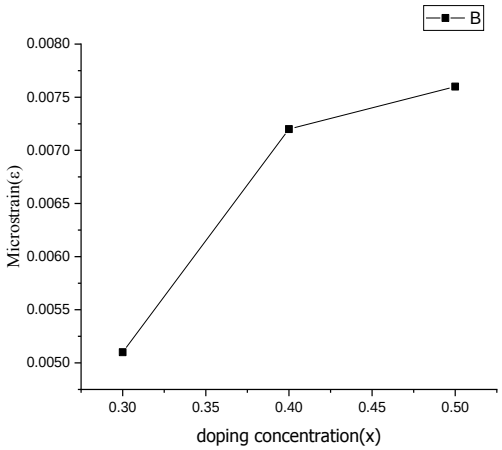

Fig 3- Variation of microstrain with doping concentration

Table1:Variation in lattice parameters,cell volume,crystallite size,microstrain for x=0.3,0.4,0.5

Doping concentration(x)	Lattice parameters		Unit cell volume V (in A^3)	Crystallite Size D (in nm)	Microstrain (ε)
	a=b (in A^0)	c (in A^0)			
0.3	5.64	13.79	379.45	24.58	0.0051
0.4	5.65	13.75	380.00	17.48	0.0072
0.5	5.68	13.89	387.80	16.62	0.0076

V- CONCLUSION

The structural analysis of barium doped bismuth ferrite samples was carried out by X-ray diffraction analysis. The X-ray diffractograms confirmed the formation of $BiFeO_3$ and also the phase purity of the synthesized samples .The decrease in the crystallite size with increasing doping concentration confirmed the distortion of the crystal. The increase in distortion of the crystal is further ascertained by the significant increase in the lattice parameters and hence the unit cell volume of the crystal as the doping concentration is increased from

x=0.3 to 0.5.The increasing values of microstrain with increasing doping concentration confirms the increasing strain induced in the lattice with increasing doping concentration of barium. In a nutshell, a small doping concentration of barium causes a significant change in the structural parameters of bismuth ferrite. This increase in the extent of distortion of the lattice with increasing doping concentrations confirmed from the values of various parameters calculated could be pivotal simply because it could lead to improved magnetization of the material. This will have huge bearing on the applications of bismuth ferrite in spintronics, sensors, microwave devices that will rule the world of communication technology in the near future.

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REFERENCES

[1] *Chaudhari,A.;Mandal,k.;(2014);"Study of structural, ferromagnetic and ferroelectric properties of nanostructured barium doped Bismuth Ferrite"; Journalof magnetism and magneticmaterials,353:57 64; DOI:10.1016/j.jmmm.2013.09.049*

[2] *T.Durga Rao, T.Karthik, Saket Asthana (2013); "Investigation of structural,magnetic and optical properties of rare earth substituted bismuth ferrite" ; Journal of Rare Earths, Vol 1; Issue 4, pp.370-375.*

[3] *M.M.El-Desoky, M.S. Ayoua, M.M.Mostafa, M.A.Ahmed (2016), "Multiferroic properties of nanostructured barium doped bismuth ferrite"; Journal of Magnetism and Magnetic Materials, 404 (68-73).*

[4] *Astita Dubey, M.Escobar Castillo, Vladimir V ,Shvartsman, Doru C.Lupascu (2019) ,"Tuning the optical, structural and multiferroic properties of Bismuth Ferrite($BiFeO_3$) Nanoparticles by Doping with Ba"; IEEE International symposium on applications of Ferroelectrics(ISAF);doi: 10-1109/ISAF 43169.2019.9034963*

[5] *Shisode, M.; Bhoyar, D; Khirade, P; Jadhav ,K(2015);"Structural, Microstructural,Magnetic, and Ferroelectric Properties Of Ba^{2+}-Doped $BiFeO_3$ Nanocrystalline Multiferroic Material" ; Applied Nanosciences, DOI:10.1007/s13204-015-04698,*

[6] *Vijaykumar Jadhav, Shude Liu, Mu.Naushad, Rajaram Mane; (2016);"Mixed phase bismuth ferrite nanoflake electrodes for supercapacitor applications"; Applied Nanoscience,6(4),511-519*

[7] *E.Mostafavi, A.Ataie (2016) ,"Fabrication and characterization of nanostructured Ba-doped $BiFeO_3$porous ceramics"; Materials Science-Poland, 34(1),pp.148-156. DOI:10.1515/msp-2016-0017.*

[8] *Simant Kumar Srivastav,Namdeo Gajbhiye (2012), "Low temperature Synthesis,Structural, Optical and Magnetic Properties of Bismuth Ferrite Nanoparticles" ;Journal of American Ceramic Society ,95[11] 3678-3682. DOI:10.1111/j.1551-2916.2012.05411.x*