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Crystal structure investigation of La doped $BiFeO_3$ multiferroics by Rietveld analysis

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Abstract
Polycrystalline materials with composition $Bi_{0.8}La_{0.2}FeO_3$ multiferroics were prepared through solid state reaction method. The room temper ature XRD confirmed the very well synthesis of the sample without any trace of any impurity phase. The Rietveld analysis of the XRD pattern manifest the interesting evident of devising the structural phase not exactly Rhombohedral (R3c) but instead it exhibits a combination of 90% rhombohedral(R3c) and 10% α phase of $BiFeO_3$ Triclinic (P1). This goes in contradiction to the previously reported studies which emphasize the structure to be restricted to rhombohedral phase. The decency of the fit can be confirmed through the lower values of Rp, Rwp, and χ^2. The density spectrum get by the G- Fourier program of FullProf predict the uniformity in sample structure. The significance of the study lies in the restriction of impurity phases while synthesis, which leads to unwanted leakage currents (losses).

Keywords: *Crystal structure, multiferroics, polycrystalline*

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INTRODUCTION
Multiferroic materials are those which exhibit more than one ferroic orders (ferroelectricity, ferromagnetism, ferroelasticity and ferro-toroidicity) simultaneously. In multiferroics materials, the coupling interaction between ferro/ferri magnetic and ferroelectric order parameters produce the new effect, termed as magneto-electric (ME) effect [1]. Such coupling between magnetism and electricity offer a broad range of potential applications in multiple state memories, magnetic sensors, transformers and microwave devices [2]. ME materials get electrically polarized when subjected to applied magnetic field and get magnetized when subjected to an external electric field. Magneto-electric phenomena are found in both composites as well as single phase materials. Single phase ME materials are rare and they show low ME output. These demerits of single phase materials demand the use of alternate materials (ME composites) to enhance the ME response. Magneto-electric response in ME composites is a result of product property of its constituent phases; while ME effect is absent in both phases. $BiFeO_3$ has been among the most attentive single phase multiferroics materials, because it has both a ferroelectric and antiferromagnetic parameters with a record high Curie and Neel temperatures (TC = 1103 K, TN = 643 K).

EXPERIMENTAL DETAILS
Polycrystalline $Bi_{0.8}La_{0.2}FeO_3$ multiferroics were synthesized by the conventional two stage solid state reaction method using high purity analytical grade Bi_2O_3, La_2O_3 and Fe_2O_3. These materials were carefully weighed in stoichiometric proportion, mixed thoroughly and ground in an agate mortar till a homogeneous mixture was formed. The compacted mixture of reagents taken in desired cation ratios was first calcined at 753 K [1–3] for 3 hours with again grinding of the powder, the final heat treatment at 800°C in air for two to three hours has been carried out. XRD patterns which were collected at room temperature using a Rigaku Miniflex-II diffractometer with Cu Kα radiation in the 2θ range (10-80°) at slow scanning rate of 2 °/min. The data was further analysed by the Rietveld refinement using FullProf program [4]. Magnetic properties were evaluated using vibrating sample magnetometer which was carried out at room temperature with a maximum applied field of 15 kOe.

RESULT AND DISCUSSION

Figure 1 represents the powder XRD patterns obtained for prepared $Bi_{0.8}La_{0.2}FeO_3$. XRD patterns of without presence of any additional secondary phase [5–6]. A comparison of XRD patterns reveals that the intensity and number of ferroelectric peaks increase with increasing content of ferroelectric in the samples. For detailed crystal structure analysis, XRD data was further analysed by Rietveld refinement using FullProf software [7]. The Rietveld analysis of XRD parameters requires that intensities, as well as the shapes of diffraction peaks, must be replicated [8]. The various parameters obtained from Rietveld refinement analysis are given in the Table 1. In order to model a crystal structure with the Rietveld refinement, we need to fit a large number of observed parameters along with crystallographic parameters [9].

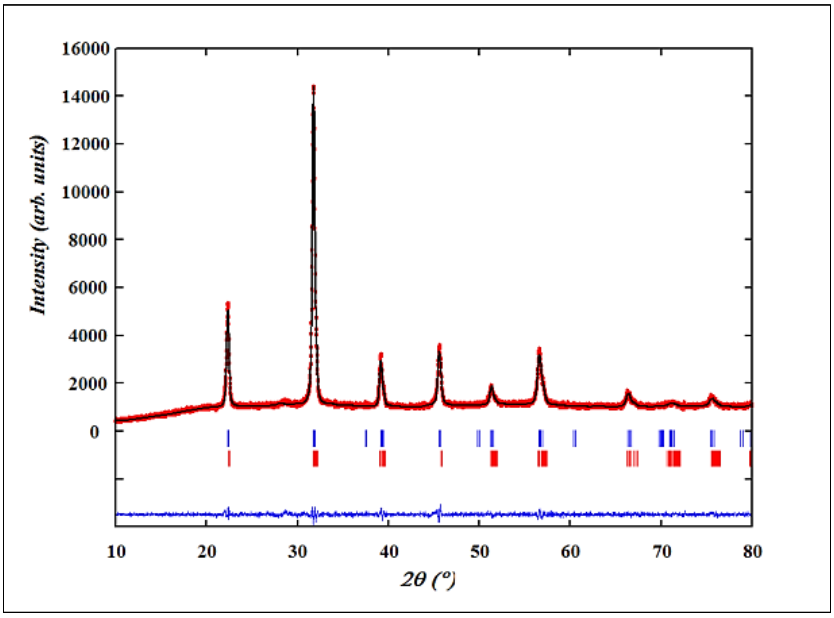

Fig. 1: *(a) Fullprof Simulated XRD Pattern of $Bi_{0.8}La_{0.2}FeO_3$ Sample.*

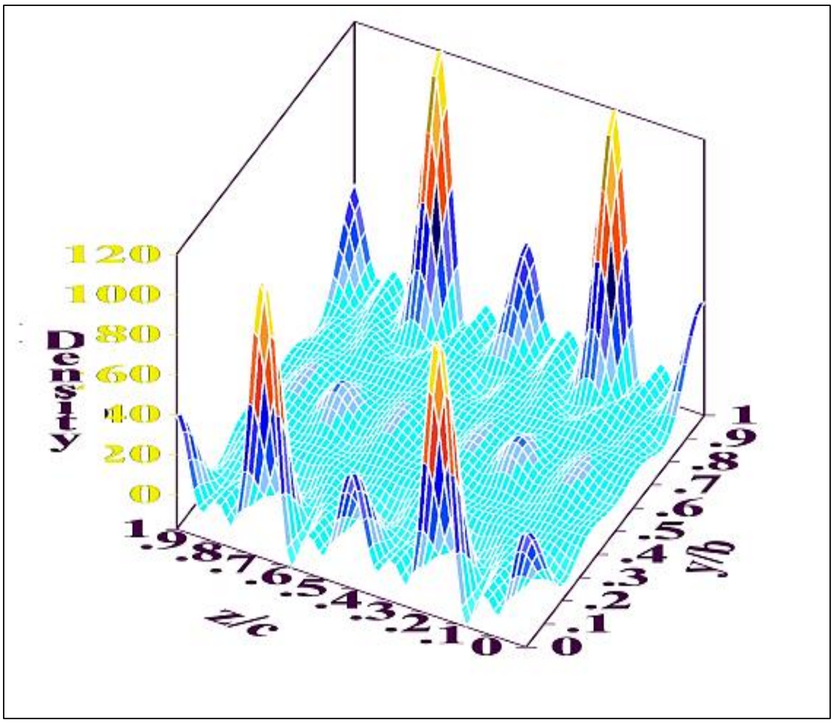

Fig. 1: *(b) Fullprof Simulated Density Spectra of $Bi_{0.8}La_{0.2}FeO_3$ Sample.*

Table 1: *Refined Parameters for Prepared Sample.*

Sample Name	Space Group	Atom	Site	x	y	z	R-factor
$Bi_{0.8}La_{0.2}FeO_3$	R3c (30.87%)	Bi/La	6a	0	0	0.224619	Rp = 3.45
	a = 5.5787	Fe	6a	0	0	0	Rwp = 4.62
	c = 13.7899	O	18b	0.88645	0.63543	0.44144	χ^2 = 3.23
	P1 (69.13%)	Bi1/La1	4g	0.69435	0.11468	0	Mag. Moment of Fe^{3+} = 4.27700 μ_B
	a = 5.5698	Bi2/La2	4h	0.71563	0.13005	0.5	
	b = 11.2360	Fe	8i	0.23925	0.12216	0.24450	
	c = 7.6088	O1	4g	0.28286	0.15433	0	
		O2	4h	0.28790	0.10232	0.5	
		O3	8i	0.06601	0.27091	0.28021	
		O4	4f	0	0.5	0.19782	
		O5	4e	0	0	0.19493	

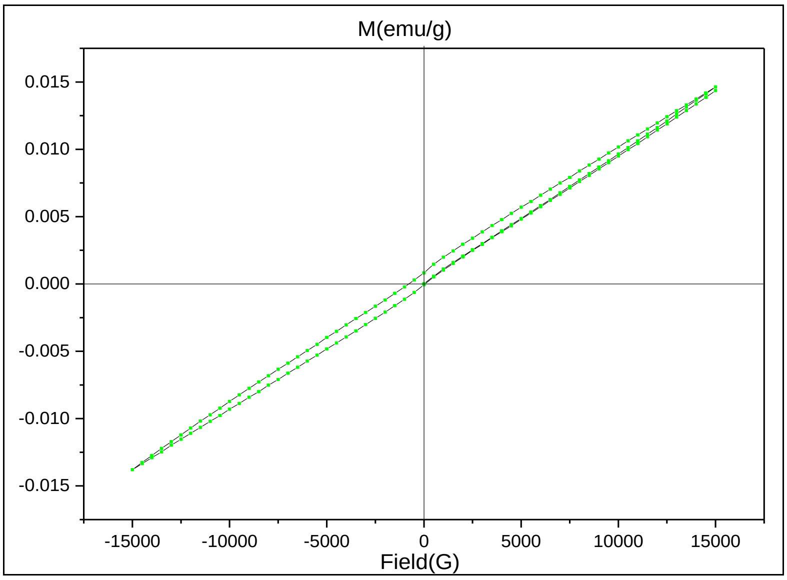

Fig. 2: *M-H Loops of $Bi_{0.8}La_{0.2}FeO_3$ Sample.*

Figure 2 shows the magnetization hysteresis (M-H) loops for substituted sample. The $Bi_{0.8}La_{0.2}FeO_3$ shows very small value of remanent magnetization which is for basic antiferromagnetic structure.

CONCLUSIONS

The low value of $\chi 2$ and profile parameters (Rp and Rwp) suggests good agreement between observed and calculated value. Enhanced magnetization is attributed to the partial structural distortion as evident by change in bond angle and bond distances. Significantly enhanced magnetization due to suppression of spin cycloid structure suggests that these material act as the promising candidate for data storage media.

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