# Structural and Optical Properties of Iron Doped Barium Strontium Titanate

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**Abstract**
Bulk samples of Iron doped at B- site in ($ABO_3$) perovskite Barium Strontium Titanate ($BaSrTiO_3$) were synthesized by Solid State Reaction Route . XRD confirmed the pure perovskite phase formation. The SEM micrographs show proper grain growth and EDAX confirmed the presence of all the elements in samples. The FTIR and Raman Spectroscopy revealed the chemical bonding and presence of new peaks with Fe doping in BST samples.

**Keywords**
Multiferroics, Barium Strontium Titanate (BST), Raman, FTIR

## I. Introduction

The term Multiferroics refers to intertwining of basic ferroic properties like ferroelectricity and ferromagnetism simultaneously in single phase perovskite materials, has attracted many researches in past few decades. Multiferroic materials have potential applications in information storage, spintronics and multistate memories. Among various perovskite materials Lead based multiferroic materials like PLZT, PZT and $PbTiO_3$ are widely investigated. But due to environmental, health and social reasons these materials are not preferred in devices and attempts are being made to replace them with environment friendly materials [1].
Barium Strontium Titanate abbreviated as $Ba_{1-x}Sr_xTiO_3$ being environment friendly, has high dielectric constant, low dissipation factor, compositional-dependent Curie temperature (Tc) and large electro-optical coefficient. BST is promising candidate to be used as phase shifters, resonators, filters and capacitors in communication systems [2-3]. It also has optical applications in non-linear optical devices such as planar waveguides or optical switches Because of low optical propagation losses [4]. In this work we have investigated structural and optical properties of $Ba_{0.7}Sr_{0.3}TiO_3$ with doping of $Fe^{3+}$ at B-site.

## II. Experimental Procedure

The Bulk Samples of Fe iron Doped BST with composition $Ba_{0.7}Sr_{0.3}Fe_xTi_{(1-x)}O_3$ where x=0, 0.1, 0.2, 0.3 (abbreviated as BST, BSTF1, BSTF2, BSTF3) were prepared using solid state reaction route. Raw materials ($BaCO_3$, $SrCO_3$, $Fe_2O_3$ and $TiO_2$) were weighed in desired stoichiometric ratio and ball milled for 6 hours. For proper phase formation Calcination was done at 1000°C for 5 hrs followed by PVA mixing (2% of weight of powder) was done. Pressing of PVA mixed powder in form of pellets was done in 10mm dye by applying pressure of 10 MPa. Sintering at 1250°C for 12 hrs for proper grain growth and densification of samples was done in programmable furnace.
The prepared bulk samples were then characterized using various techniques. Structural Characterization was carried out using Room temperature X-Ray Diffraction ($CuK_\alpha$ radiation, SHIMADZU MAXima XRD -7000) , Scanning Electron Microscope (FESEM) (Carl ZEISS Supra 55) and Energy dispersive X Ray analysis (EDAX) (OXFORD instruments attached with FESEM). The optical properties FTIR and Raman Spectroscopy were studied by PERKIN-ELMER Fourier Transform spectrophotometer and RENISHAW inVia Raman microscope.

## III. Results and Discussions

### A. Structural Properties

The phase formation, microstructure and elemental composition studied for BST samples is discussed below in following sections

### 1. Phase Formation

X-Ray diffraction patterns of sintered powder taken at room temperature showing sharp peaks revealed the polycrystalline perovskite phase formation. Fig. 1. Shows the XRD pattern taken for BST samples named BST, BSTF1, BSTF2 and BSTF3 corresponding to composition $Ba_{0.7}Sr_{0.3}Fe_xTi_{(1-x)}O_3$ where x=0, 0.1, 0.2, 0.3

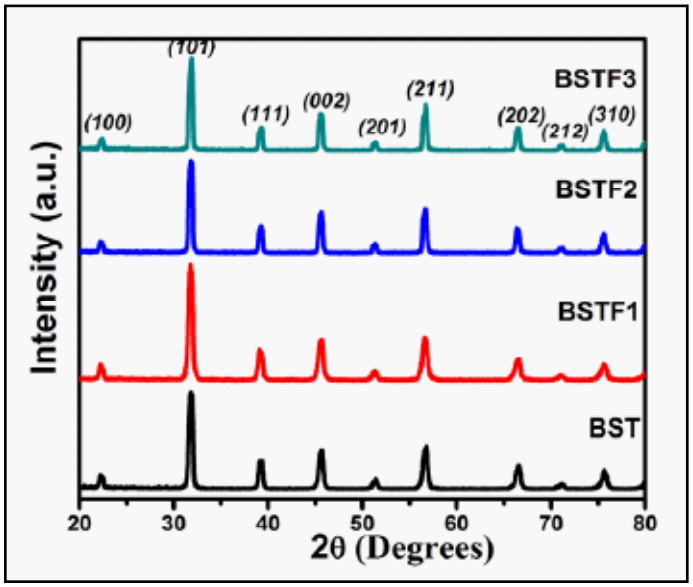



Fig. 1: XRD Pattern of Sintered BST Samples (a) BST (b) BSTF1 (c) BSTF2 (d) BSTF3

The peaks indexed to (100), (101), (111), (002), (201), (211), (202), (212) and (310) confirms the Barium Strontium Titanate `s perovskite phase which are in good agreement with literature results [1-2, 4-5]. BST and BSTF1 have tetragonal structure and BSTF2 and BSTF3 have cubic structure. An obvious shift in peaks is observed with doping of Fe in BST.

### 2. Microstructure

The SEM micrographs of sintered pellets were taken at same magnification of 10KX to study the surface morphology in all BST samples. The SEM images of Sintered Samples are shown in fig. 2.

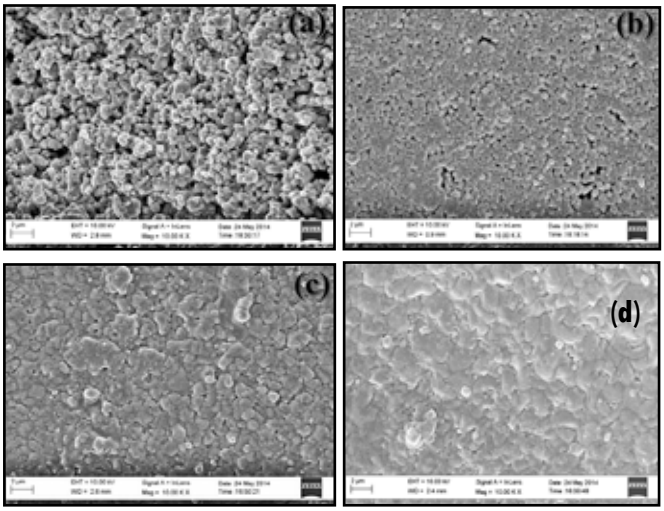



Fig. 2: FESEM Images of (a) BST (b) BSTF1 (c) BSTF2 (d) BSTF3

The images clearly show grain growth in all the samples. With doping of iron BSTF1 appears to be much denser than BST and BSTF3 appears to be bit denser than BSFT2. The average grain size was estimated for the broadening of (101) peak from the full width half maximum (FWHM) using Debye Scherrer Formula

$$B(2\theta) = \frac{K\lambda}{L\cos\theta}$$

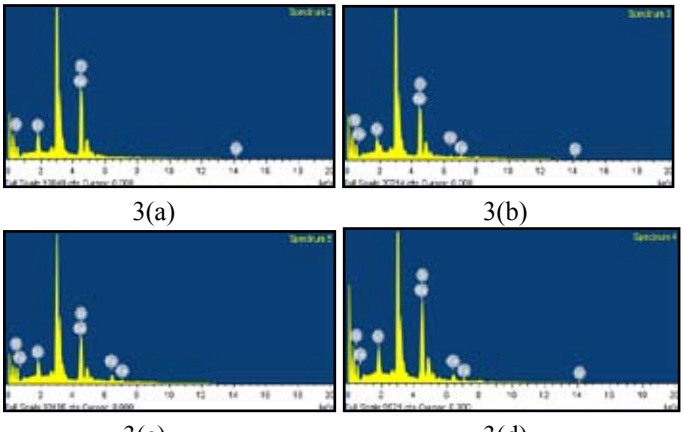
where B is Peak width, $\lambda = 1.54A^{o}$ and , K is the Scherrer constant, L is estimated grain size. The density of bulk samples calculated using Archimedes principle and the estimated grain size from Debye Scherrer Formula appears to be following the same trend which is shown in table 1. Below.

Table 1: Grain Size and Bulk Density Variation of BST Samples (a) BST (b) BSTF1 (c) BSTF2 (d) BSTF3

| Sample Name | Grain Size (nm) | Bulk Density (g/cc) |
|---|---|---|
| BST | 514.43 | 5.282 |
| BSTF1 | 844.26 | 6.301 |
| BSTF2 | 253.63 | 5.424 |
| BSTF3 | 1289.14 | 5.627 |

## 3. Composition

The Energy Dispersive X- Ray Spectra confirmed the presence of main elements (Ba, Sr, Ti) and doped element (Fe) in all the samples as shown in fig. 3. The weight% of all elements is shown below in Table 2.



3(a) 3(b)

3(c) 3(d)

Fig. 3: EDAX Spectra of (a) BST (b) BSTF1 (c) BSTF2 (d) BSTF3

Table 2: The Weight % of all BST Samples (a) BST (b) BSTF1 (c) BSTF2 (d) BSTF3

| Sample | %Ba | %Sr | %Fe | %Ti |
|---|---|---|---|---|
| BST | 57.32 | 15.31 | ------- | 27.37 |
| BSTF1 | 64.62 | 14.02 | 2.62 | 18.73 |
| BSTF2 | 55.33 | 17.51 | 6.30 | 20.86 |
| BSTF3 | 55.90 | 16.54 | 10.06 | 17.50 |

## B. Optical Properties

FTIR and Raman Spectroscopy are studied for BST samples are discussed below in following sections

## 1. FTIR Spectroscopy

The Infrared Spectra (IR) was measured using KBr pellets made from mixture of sintered powder of Fe doped BST samples. The IR spectra for all the samples were measured from 450-2000 $cm^{-1}$. The observed spectra are shown in fig. 4.

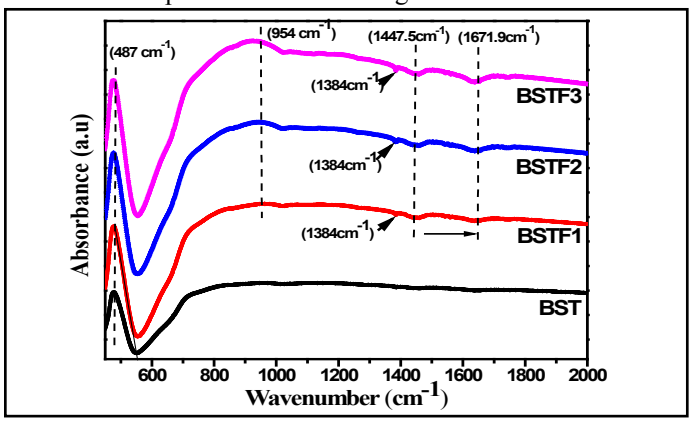



Fig. 4: FTIR Spectra of (a) BST (b) BSTF1 (c) BSTF2 (d) BSTF3

The observed IR spectra for all the samples show a prominent peak at 487 $cm^{-1}$,which corresponds to Ti-O stretching vibrations in all the samples.[6] This peak corresponding to Ti-O stretching appears be getting more intense with increase in Fe doping. A shoulder around 954$cm^{-1}$, a dip at 1384$cm^{-1}$ and band in region 1447$cm^{-1}$-1671$cm^{-1}$ appears to be getting more prominent in Fe doped BST samples corresponding to formation of new bonds due to dopant (Fe).

## 2. Raman Spectroscopy

The Raman spectra was measured from 50-1500 $cm^{-1}$ for Fe doped BST samples (pellets) with laser wavelength of 488 nm and excitation time of 30 sec.

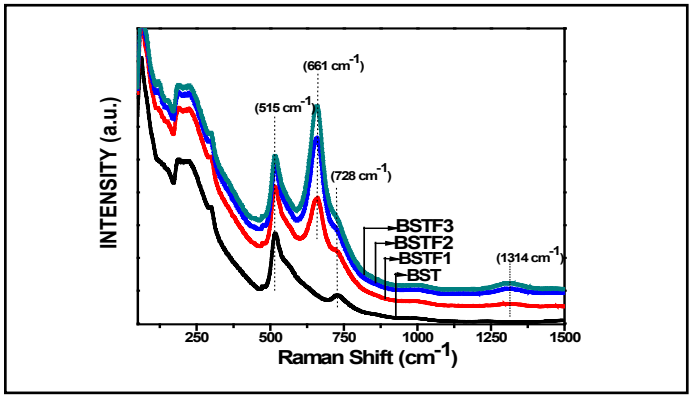



Fig. 5: Raman Spectra of (a) BST (b) BSTF1 (c) BSTF2 (d) BSTF3

The Raman Spectra of the BST samples is shown in fig. 5. The vibrations around 515 $cm^{-1}$ and 728 $cm^{-1}$ may be attributed to A1TO and A1LO mode corresponding to change of the Ti-O-Ti bond angle [7]. A sharp Peak at 616 $cm^{-1}$ and a broad peak at 1314 $cm^{-1}$ appears with addition of dopant (Fe). These both peaks are getting more intense with increase of Fe concentration in BST samples.

## IV. Conclusion

$Ba_{0.7}Sr_{0.3}Fe_xTi_{(1-x)}O_3$ ceramics with x=0, 0.1, 0.2, 0.3 were prepared using solid state reaction route. The structural analysis using XRD and SEM revealed perovskite phase and proper grain growth respectively in all samples. EDAX confirmed the stoichiometry of all the samples. In FTIR and Raman spectra the new peaks confirmed the formation of bonds due to doping of Fe in BST samples.

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