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Synthesis and structural analysis of Barium Samarium Zirconium Titanate (BSZT)

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Abstract : *Barium Samarium Zirconium Titanate (BSZT) was synthesized by doping samarium on the A sites of barium zirconium titanate (BZT). BSZT was prepared by dry route method. For BSZT raw materials were taken in stoichiometric proportion and placed in ball mill for 72 hrs for homogeneous mixing and then calcinations was done at 1300°C .Lumps were then grinded and XRD of the calcinated powder were done. Pellets were made and sintered at 1350°C. Poling and Electroding was done for characterization. Poling and electroding are required to form the capacitor. The diffraction peaks of the samples were shifted to the higher angle side with the increase of samarium doped concentration.*

Key Words : *XRD, Doping, Sintering, calcinations, poling.*

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Introduction :

Ferro electricity is a property of certain materials which has spontaneous polarization that can be reversed by the application of an external electric field. It has also been called seignette electricity, as seignette or Rochelle salt was the first material found to show ferroelectric property such as spontaneous polarization on cooling below curie temperature, ferroelectric domains & ferroelectric hysteresis loops (Dekker 2010).

Due to environmental concerns, there has been growing interest in the use of lead free ceramics such as Barium Titanate (BT) and BZT in applications such as sensors and actuators. Barium Titanate ($BaTiO_3$) is an electric insulator in pure form. Barium Titanate has a paraelectric phase above its curie point(T_c) of about 120°C. At T_C it undergoes phase change from tetrahedral to cubic. Barium titanate as a powder white to grey in colour has a perovskite structure. It is insoluble in acid like H_2SO_4, HCL, and HF and soluble in alkali and water. It can be manufactured by liquid phase sintering of barium carbonate and titanate dioxide optionally with other materials for doping. (Haertling 1999).

Barium zirconium titanate is the most attractive one because it is derived from two perovskite lattice i.e, Barium Titanate ($BaTiO_3$) and Barium Zirconium ($BaZrO_3$) which have been reported that the zirconium substitution into the titanium lattice enhance the dielectric and piezoelectric properties. Zr-doped BZT ceramics exhibit typical diffuse paraelectric to ferroelectric phase transition behaviour in which T_c (curie temperature) shifts to higher temperature with increase of frequency. $Ba(Zr_xTi_{1-x})O_3$ is an important member of the $BaTiO_3$ based ferroelectric materials family which presents higher voltage resistance characteristics. BZT ceramics are attractive candidates for dynamic random access memories (DRAM) and tunable microwave devices (Maiti et al 2011).

Barium samarium zirconium titanate, BSZT ($Ba_{1-x}Sm_xZr_{o.15}Ti_{o.85}O_3$) is a ferroelectric ceramics formed by doping Sm^{3+} ions on the A sites of barium zirconium titanate (BZT). It has same perovskite structure as BZT and BT(Sagar et al 2011) .

In barium samarium zirconium titanate (BSZT), formed by doping Sm^{+3} ions on the A site of BZT, Sm^{+3} is a rare earth element and it is seen that doping of ceramics with rare earth oxide of Sm, shifts the curie point to lower temperature (Moura et al. 2008).

We report the synthesis and structural analysis of BSZT sample and the effect of doping of Sm^{+3} ion in different amount(x=0.00, x=0.02, x=0.03) in the samples in this paper. We find the dry route method for the preparation of ceramics as a low cost effective method.

Materials and Methods:

There are various methods used for preparation of samples. Here we use dry route method (Nierman 2011). After preparing the samples electroding and poling were done. The chemicals used for the samples ($Ba_{1-x}Sm_xZr_{o.15}Ti_{o.85}O_3$) where x=0.00, 0.02, 0.03. The weighed compounds $BaCO_3$(99%), Sm_2O_3(99.9%), ZrO_2(99%) and TiO_2(99%) were taken in stoichiometric proportion and put in nylon bottle and acetone and few zirconium balls were added to it. The mixture was placed in ball mill for 72 hours. Then the samples were placed in an oven for nearly 2-3 days at a temperature of 50°C .After that the zirconium balls were removed from that sample. The obtained samples were placed in a muffle furnace for 4 hours at 1300°C in a closed alumna crucible for calcinations. By the calcinations, oxygen from the sample were removed which resulted in the formation of lumps of sample. The samples were grinded in Agate mortar pestle to break the lumps properly by adding acetone in small quantity. The powder form of the samples were ready for the XRD by Miniflex –II. Then the pellets(10 mm) of all the three samples of ($Ba_{1-x}Sm_xZr_{o.15}Ti_{o.85}O_3$) where (x= 0.00, x=0.02, x=0.03) were prepared by Dipunch machine at a pressure of 7 ton from hydraulic pressure machine. The pellets were sintered at 1350°C for two hours in high temperature furnace. After that the upper and lower surface of pellets (Fig 1) were coated with silver paint for electroding and poling and then put in furnace at 50°C for two hours. The XRD patterns were recorded using X-Ray Diffraction machine (Miniflex-II).

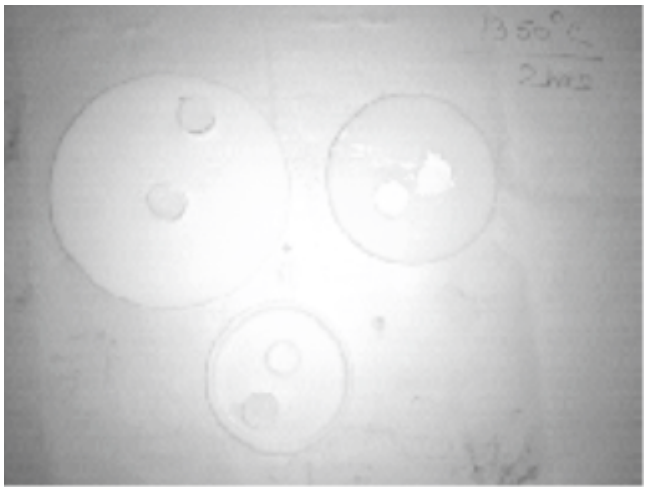

Fig 1 : Pellets of BSZT samples

Results and Discussion :

It was observed that the diffraction peaks of samples shifted to a higher angle side with the increase of samarium doped concentration (Table 1). It can be explained by noting that doped Sm^{3+}ions occupy the A sites of barium zirconium titanate oxide lattice structure. The phase transition peaks (Fig 2) seem to be sharper in case of undoped BZT than those of samarium doped BZT. The substitution of Sm^{3+} ions at A sites of Ba^{2+}ions is for maintaining the perovskite structure of solid solution and resulting in the disorder distribution of A sites ions. Therefore the chemical inhomogeneity of $(Ba_{1-x}Sm_x)\ Zr_{0.15}Ti_{0.85}O_3$ ceramics and the distortion of the lattice of perovskite structure ABO_3 are originated (Kumari et al 2013).

Table 1. Calculation from XRD

Sample $Ba_{1-x}Sm_xZr_{0.15}Ti_{0.85}O_3$	Particle size(Å)	hkl value	Interplanar distance (Å)	Braggs angle, θ (degrees)	Lattice constant
x=0.00	335	200	2.3280	19.32	4.65
x=0.02	288	200	2.0176	22.445	4.0352
x=0.03	279	200	2.0221	22.34	4.044

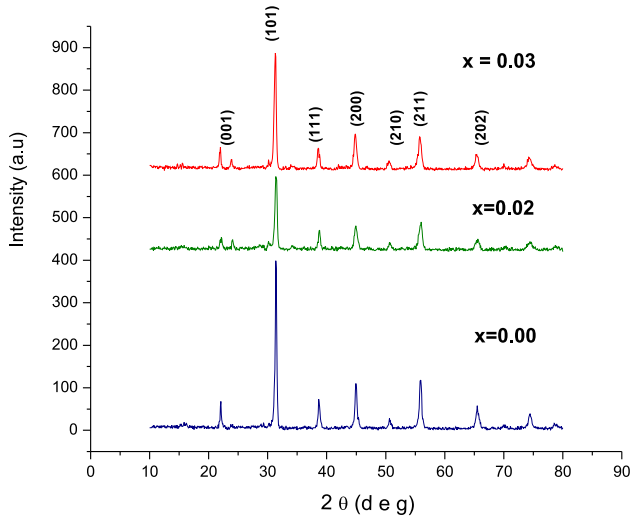

Fig 2 . Comparative study of XRD pattern of BSZT samples

Reduced lattice parameter of the BSZT samples were obtained after substitution of Samarium in BZT. There was a gradual shift of peaks of samples. They were shifted to the higher angle side with the increase of samarium doped concentration.

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