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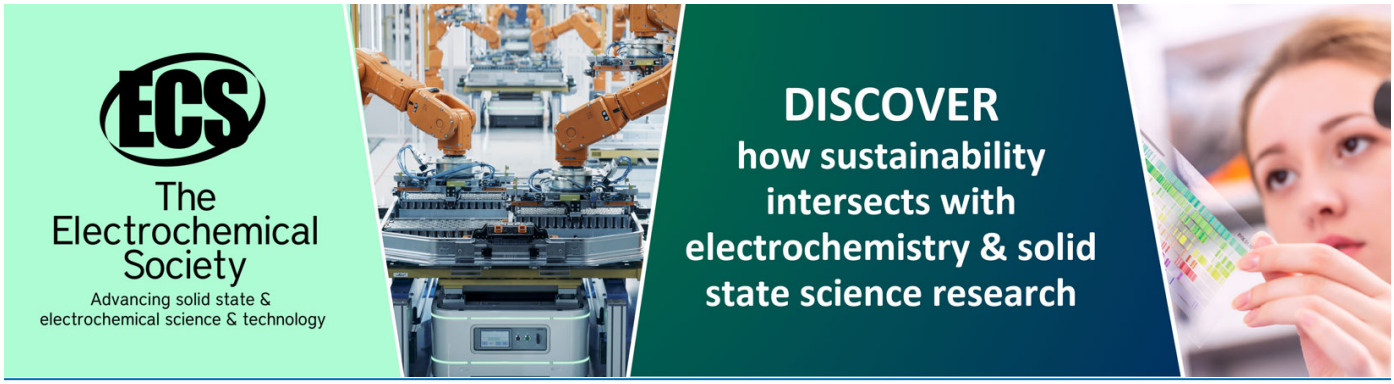

Synthesis, Structural and Electrical Properties of $Y_{1-x}Ca_xFeO_3$ (X= 0.03 and 0.05) Ceramics

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Abstract. The single-phase ceramic samples of Perovskite $Y_{1-x}Ca_xFeO_3$ (YCFO) were synthesized successfully by solid state reaction method. The prepared samples of YCFO were analyzed by room temperature X-ray diffraction techniques and the data were fitted with FullProf program which confirmed the orthorhombic symmetry with Pnma space group. To estimate electrical parameters the samples were analyzed by I-V and dielectric measurement techniques and observed that the overall conductivities enhances with increase in temperature as well as with doping concentration.

Keywords:- Solid state reaction, X-ray diffraction, Dielectric constant, Semiconductor

1. Introduction

Multiferroic Perovskite materials attract interest of researcher's community for its unusual behaviour and interesting physical properties and hence play an important role in technical applications like electrode materials, sensors, catalysts etc. [1-5]. $YFeO_3$ is one such type of multiferroic Perovskite which possesses high magneto-optical figures of merits in the near IR regions and high domain wall velocity and hence it is very useful in memory storage and magneto-optical devices [6-8]. $YFeO_3$ has high electrical resistance and hence its conductivity is not good enough which has been reported in our previous paper [9]. The conductivity of $YFeO_3$ can be improved by the addition of CaO up to a certain amount which makes this material suitable for electrode material [10-12]. Hence Ca doped $YFeO_3$ is a potential candidate as cathode material in solid oxide fuel cells due to its high electrical conductivity and good thermal stability at high temperature. From the review of literature [13-15] it is observed that $YFeO_3$ has not been studied much and there is no systematic report available on the structural and electrical properties of this compound. The present paper reports on synthesis, structural and electrical properties of Calcium substituted $YFeO_3$ ceramics.

2. Experimental procedure

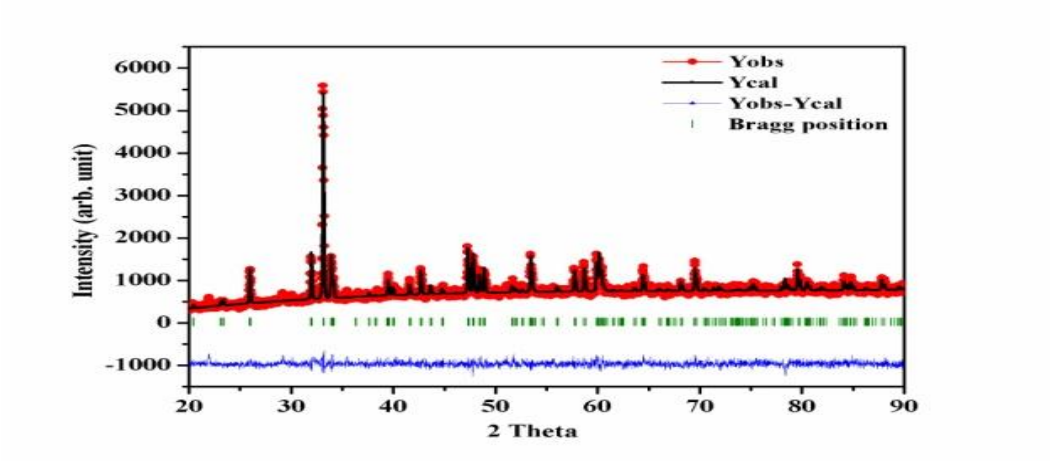
Analytically Y_2O_3, CaO and Fe_2O_3 (with high purity 99.99%) were used as raw materials in the fabrication of Perovskite YCFO ceramics using high temperature solid state reaction method. These raw materials were mixed in stoichiometric amount and grinded in agate mortar up to 6 hours in the presence of a binding agent (acetone). The grinded powders were calcined. This process of grinding and calcination was repeated for a number of times between the temperature ranges from 973K to1473K. These prepared powders were pressed in a die of 10mm by applying the pressure approximately 5tons/cm^2 to convert in to pallet form. These pallets were finally sintered at 1573K for 6hrs.The formation and structure of these compounds were examined by room temperature X-ray diffraction technique using Rigaku (model:- Ultima-IV), X-ray diffractometer in 2θ range from 20^0 to 90^0. The important structural parameters like lattice

constant, miller indices etc. were obtained using Rietveld fitting of XRD profile with the help of FullProf program. The I-V measurement at various temperatures (RT to 573K) were carried out for both of the samples in the positive as well negative voltage range from -5Volt to +5Volt, using the Source meter (model:- Agilent B2901A) and laboratory made furnace setup. The AC conductivity measurement was carried out using the LCR meter (model: - HIOKI 3532-50 LCR Hi-Tester). The dc conductivity was also measured by two probe method using the laboratory made setup. The results are discussed in detail.

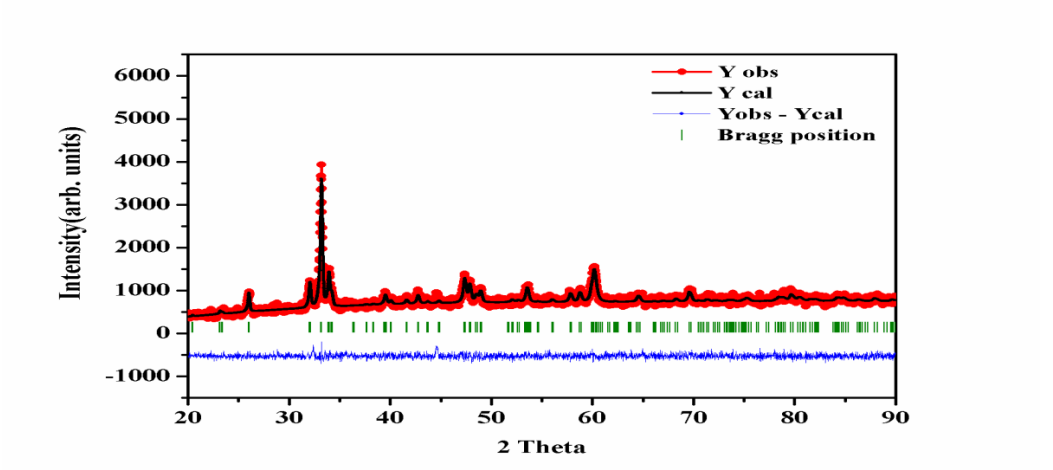
3. Results & Discussion

3.1 Structural analysis

The Rietveld refinement profile of $Y_{1-x}Ca_xFeO_3$(x=0.03 and 0.05) are shown in Figure 1(a & b) which shows the orthorhombic symmetry with space group Pnma. No impurity peak was observed in the diffraction pattern which confirmed that the formation of compounds has been completed during synthesis process. There is a good agreement between the observed and fitted profile. The detailed parameters related to its structure obtained from Rietveld refinement technique are presented in Table 1. The value of χ^2 is not high which also confirmed that observed and calculated values are in good agreement for both samples.



(a)



(b)

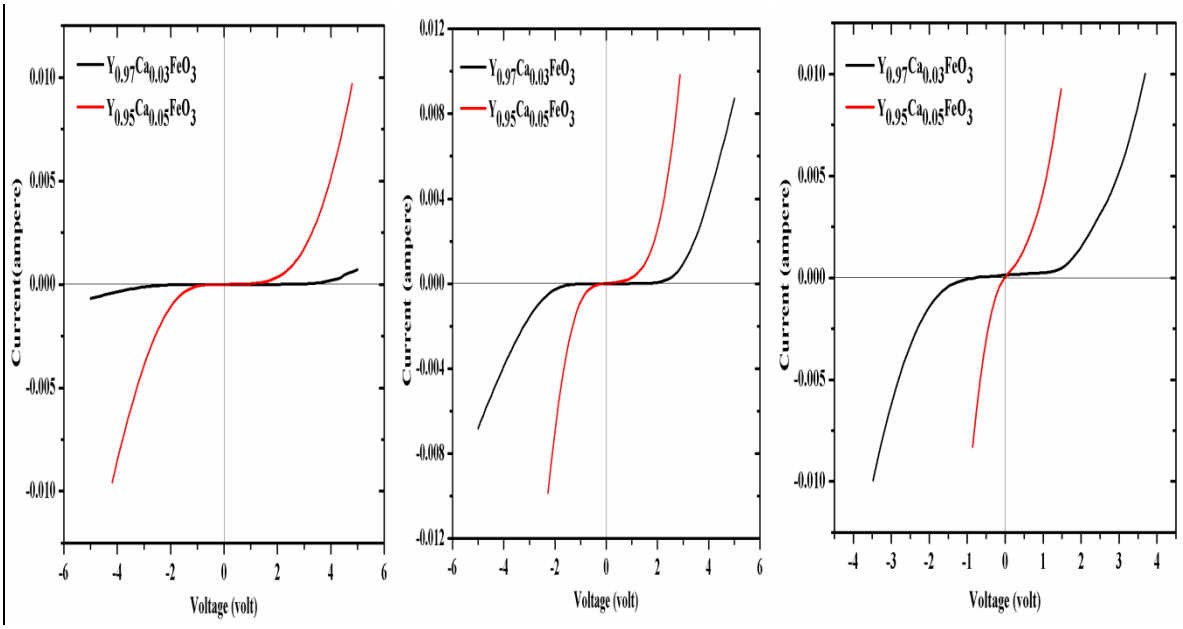
Figure 1(a & b). Rietveld Refinement profiles of $Y_{1-x}Ca_xFeO_3$(x=0.03 and 0.05).

Table: 1 Detailed Structural parameters of $Y_{1-x}Ca_xFeO_3$ (x=0.03 and 0.05) obtained from Rietveld Refinement of X-ray powder diffraction pattern.

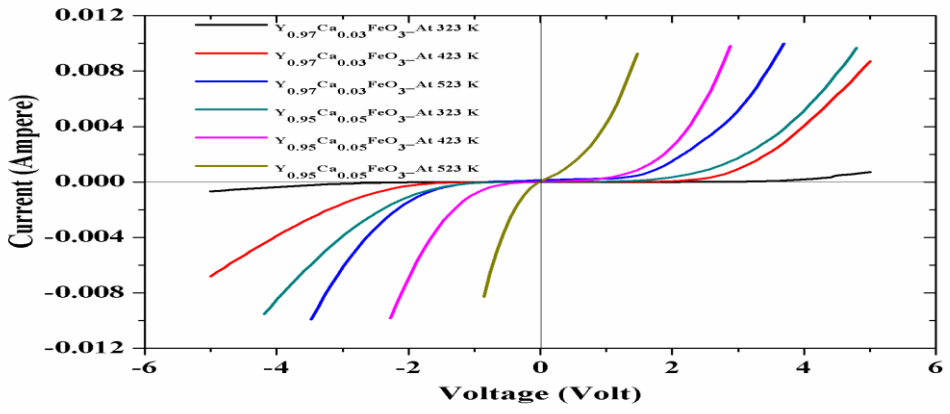
Parameters	X = 0.03	X = 0.05
2Θ Range(degree)	20 - 90	20 – 90
Step Size(degree)	0.02	0.02
Crystal symmetry	Orthorhombic	Orthorhombic
Space group	Pnma	Pnma
Centro-symmetric	Centric	Centric
Cell parameters(Å)		
a	5.5922	5.5849
b	7.6038	7.6000
c	5.2833	5.5828
Unit cell volume($Å^3$)	224.6558	224.3537
Number of data points	3501	3501
Half width parameters(degree)		
U	0.02878	-0.01387
V	-0.00512	0.15486
W	0.03032	0.01860
Number of reflections	102	111
Bragg R – factor	15.7	8.09
Rf - factor	18.8	8.17
χ^2	4.34	3.63
GOF	2.1	1.9

3.2 Electrical analysis

Figure 2 shows the I-V characteristics as a function of substitution concentration of Ca and temperature. Figure 2 (a, b & c) are showing the change in the behaviour of current with increase in voltage of $Y_{1-x}Ca_xFeO_3$(x=0.03 and 0.05) at different temperatures. In all the Figures 2 (a, b & c) the value of current for x= 0.05 is higher than the value x= 0.03, which shows that the conductivity is increasing with increase in doping concentration. From the comparison of all three figures as shown in Figure 2(d), it is noticed that the conductivity is also increasing with the increase of temperature which reflects the semiconducting behaviour of the materials.



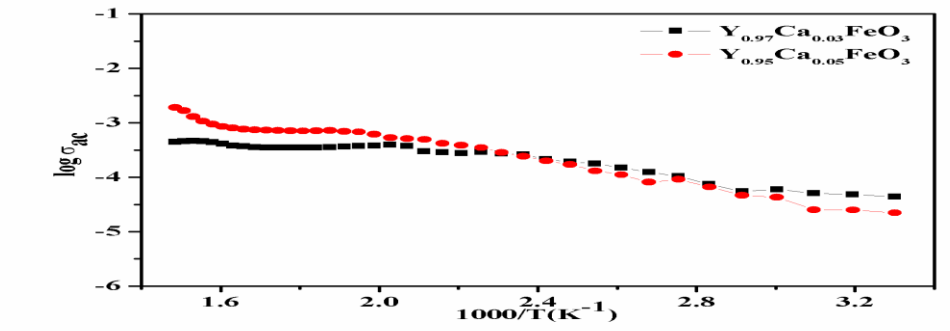
(a) At 323K (b) At 423K (c) At 523K



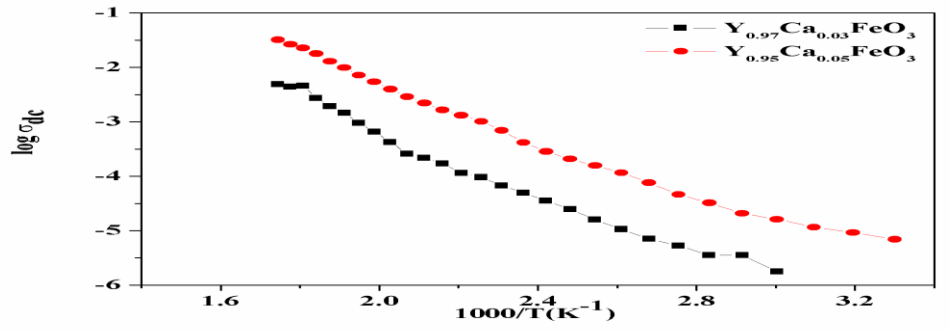
(d) Combined curve at 323K, 423K & 523K

Figure 2. I-V Characteristics curves of $Y_{1-x}Ca_xFeO_3$ (x=0.03 and 0.05).

The ac conductivity was calculated from dielectric loss measurement using the formula **$\omega = 2\pi f\varepsilon_0\varepsilon$"** (where ε_0 is the permittivity of free space and ε" is the dissipation factor) at 5 MHz and are shown in Figure 3(a). Also the dc conductivity was calculated using the Arrhenius relation $\sigma = \sigma_o \exp(-E_a/kT)$ using two probe method and are shown in Figure 3(b). It is clear from Figure 3 (a & b), that both the conductivities (ac and dc) are increasing with respect to temperature for both compounds, which reflects the semiconducting behaviour of the materials and are consistent with I-V results. Also, these conductivities (ac & dc) are increasing with the enhancement in doping concentration on A-cation site.



(a)



(b)

Figure 3 (a & b). log (σ_{ac}) and log (σ_{dc}) vs. 10^3/T curves of $Y_{1-x}Ca_xFeO_3$(x=0.03 and 0.05).

4. Conclusion

The Perovskites YCFO were prepared by solid state reaction method. The formation of the compounds as well as structure was checked by Rietveld refinement technique using the program FullProf which confirmed that both the materials show orthorhombic symmetry with space group Pnma. The prepared samples were characterized by I-V measurement techniques. The I-V curves of x= 0.03 and 0.05 at different temperatures show that conductivities are improving/enhancing with increase of calcium amount and temperature also. The ac conductivity was measured using LCR Hi-Tester for both the samples (x= 0.03 and 0.05). Also the dc conductivity was measured using the two probe method which is consistent with ac conductivity for both cases (x= 0.03 and 0.05). Both ac and dc conductivities are increasing with respect to temperature as well as doping concentration.

5. References

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