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Dielectric studies of Fe Doped SmCrO3 Perovskites

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Abstract. Polycrystalline Fe doped $SmCrO_3$ perovskite ceramics were prepared by sol-gel route and characterized by X-ray diffraction (XRD), Scanning electron microscopy (SEM), dielectric and Impedance measurements. Single-phase perovskite Fe doped $SmCrO_3$ obtained has been confirmed from the XRD pattern with orthorhombic structure. The dielectric properties of perovskite Fe doped $SmCrO_3$ ceramics were studied in the frequency range of 100Hz - 1MHz in the temperature range from 80 K to 300 K. These materials exhibited colossal dielectric constant value of ~ 10^4 at room temperature. The response is similar to that observed for relaxor-ferroelectrics. To get the detailed information, IS data analysis was performed.

1. Introduction

Materials with high dielectric constant and low dielectric loss are of technological importance in the microelectronics industry as they enable device miniaturization. In recent years, materials exhibiting a so called giant dielectric constant have been reported [1-5]. Right from the time this effect was first observed in $CaCu_3Ti_4O12$ (CCTO), attention has been concentrated on materials with perovskite structure (ABO_3), due to the set of specific properties belonged to these materials. Fe doped $SmCrO_3$ (SFCO) materials are semi conductive in nature at room temperature and conductive at high temperatures. In this paper we report details concerning the dielectric response of $SmCr_{1-x}Fe_xO_3$ (x = 0, 0.4, 0.6, 1) (SCFO) as a function of frequency and temperature along with the possible underlying mechanisms.

2. Experimental

Polycrystalline powders of SCFO were prepared by the citric acid route. The powders were annealed at 650 ^oC for 2 hours with intermediate grindings. Circular pellets were pressed at 4000 Kg/cm^2 in uniaxial disc. These pellets were sintered at 1200 ^oC for 4 hours.

Phase purity of sintered pellets was characterized by X-ray diffraction (XRD) using SHIMADZU XRD - 7000 using monochromatic Cu – Kα radiation. Cation ratios were measured using EDAX. Microstructure and the grain size distribution of the sintered pellets were studied using a SEM HITCHI S-3400 N. The surface layer of the sintered pellets was removed by grinding both sides before carrying dielectric measurements. The dielectric constant measurements were carried out in the 100 Hz – 1 MHz frequency range at various temperatures between 80 K to 300 K using HP- 4284A LCR meter and Lakeshore temperature controller with a computer controlled program.

3. Results and Discussions

The XRD patterns obtained at room temperature of the polycrystalline SCFO synthesized by citric acid method are shown in figure 1. It is observed that the XRD spectrum is of a single phase SCFO. All the peaks could be indexed to orthorhombic cell associated with space group Pbnm. The lattice parameters are given in the table 1.

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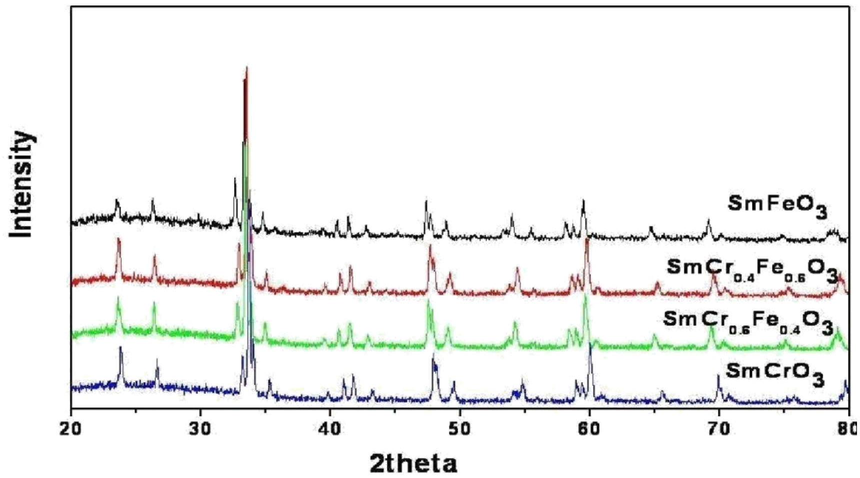

Figure 1. The XRD patterns obtained at room temperature of the polycrystalline $SmCr_{1-x}Fe_xO_3$ (x= 0, 0.4, 0.6, 1) ceramics.

Table 1. Lattice parameters of $SmCr_{1-x}Fe_xO_3$(x= 0, 0.4, 0.6, 1) ceramics.

Sample	a (A⁰)	b (A⁰)	c (A⁰)
$SmCrO_3$	5.373 (3)	5.505(2)	7.655(3)
$SmCr_{0.4}Fe_{0.6}O_3$	5.393(1)	5.544(2)	7.687(2)
$SmCr_{0.6}Fe_{0.4}O_3$	5.404(2)	5.571(3)	7.703(2)
$SmFeO_3$	5.409(2)	5.592 (1)	7.718 (2)

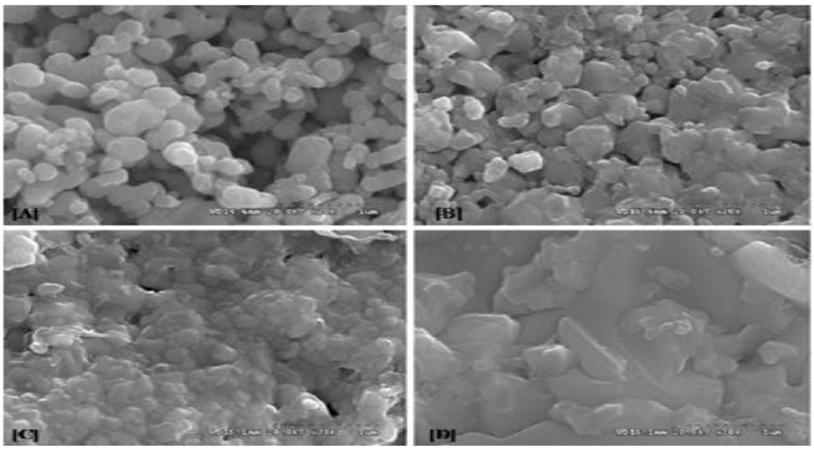

Figure 2. SEM micrograph of the $SmCr_{1-x}Fe_xO_3$ (x= 0, 0.4, 0.6, 1) pellets

The SEM micrograph of the SCFO pellets shown in the figure 2. The microstructure reveals that the pellets contain small grains with considerable porosity and as the Fe content increases the porosity is decreasing and particle size is increasing from 300 nm to 500 nm.The figure 3 and figure 4 presents the temperature dependence of the plots of the complex permittivity (ε') and loss tangent (tanδ = ε''/ε'). It is observed that ε' vs T plots exhibit similar behaviour as that of CCTO, i.e., near room temperature ε'(T) reaches a value as high as 10^4, where the ε'(T) is independent of temperature. With decreasing temperature, ε'(T) displays step like decrease to a lower value of about 7. Below 100K, ε'(T) is almost frequency and temperature independent. The step like increase in ε'(T) consists of two distinct transitions corresponding to two respective peaks in tanδ (T), shifting to high temperature as the measuring frequency increases. This indicates that there exist two sets of thermally activated relaxations in SCFO ceramic sample. It can also be seen that there is an exponential-like increasing background in tan δ curve. It is important to note that the exponential increasing background in loss tangent is associated with the hopping conductivity. This strongly suggests that the observed relaxations might be related to hopping between spatially fluctuating lattice potentials not only produce the conductivity but also give rise to dipolar effects [6].

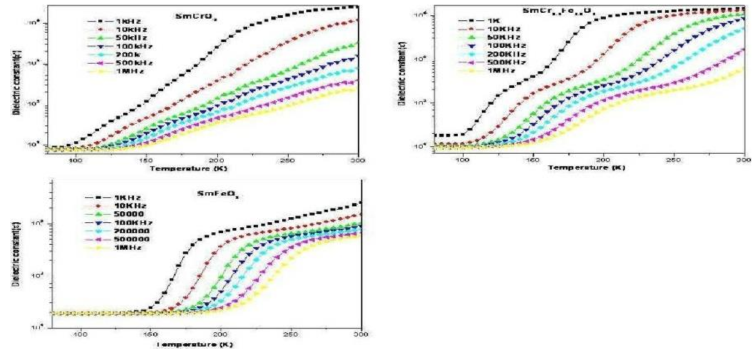

Figure 3. Temperature dependence of the permittivity (ε') of the $SmCr_{1-x}Fe_xO_3$ (x= 0, 0.4, 0.6, 1) ceramics

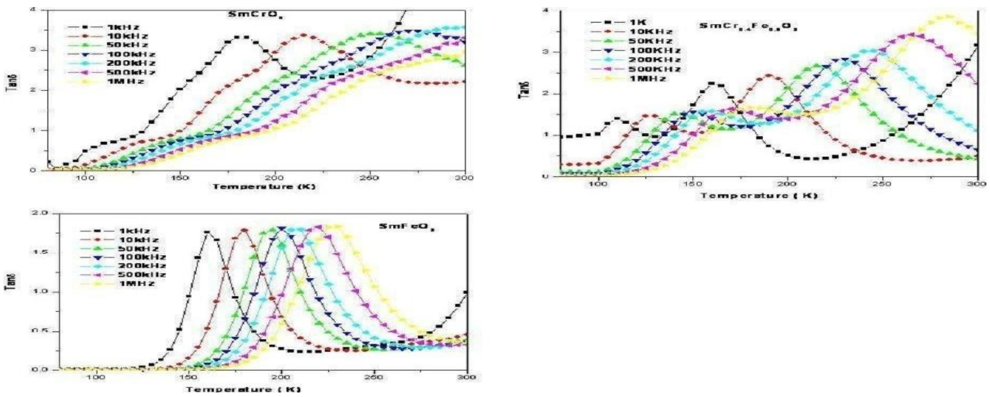

Figure 4. Temperature dependence of the loss tangent (tan δ) of the $SmCr_{1-x}Fe_xO_3$ (x=0,0.4,0.6,1.0) ceramics.

The above discussion suggests that the dielectric behaviour of SCFO ceramics is associated with the carrier polarization. Therefore the dipolar effects of hopping carriers in the grain, IBLC effects related to grain boundary and interfacial effect of electrodes are expected to be responsible for the relaxations observed in figure 4. To clarify this speculation we performed impedance analysis which enables us to distinguish different dielectric relaxations from intragrains, intergrains and electrodes of ceramic material [7-8]. The figure 5 shows an alternative presentation of Z' vs Z''/f at 160 K (5a) and 260 K (5b) as proposed by Abrantes et al [9]. Three well defined regions at 260 K are

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clearly seen in figure 6. Two regions at 160 K are observed in figure 5. According to Abrantes et al [9] these sequential regions, at 260 K, from low to high frequencies correspond, to the dielectric response from electrodes, grain boundaries and bulk grains respectively, and at 160 K grain boundaries and grain and the electrode effects are not

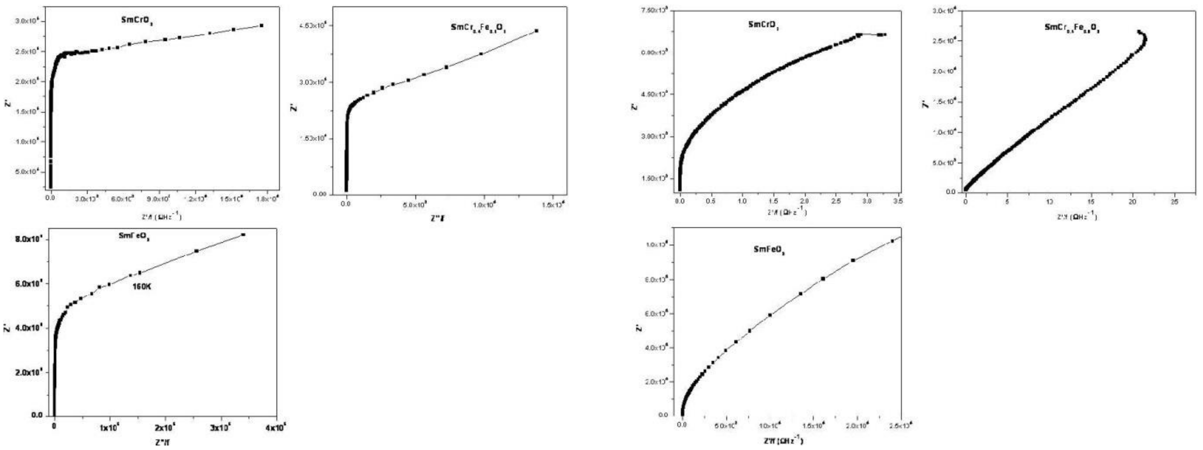

Figure 5. Representation of Z' vs Z''/f at 160 K (5a) and 260 K (5b) for the $SmCr_{1-x}Fe_xO_3$ (x= 0, 0.4, 0.6, 1) ceramics.

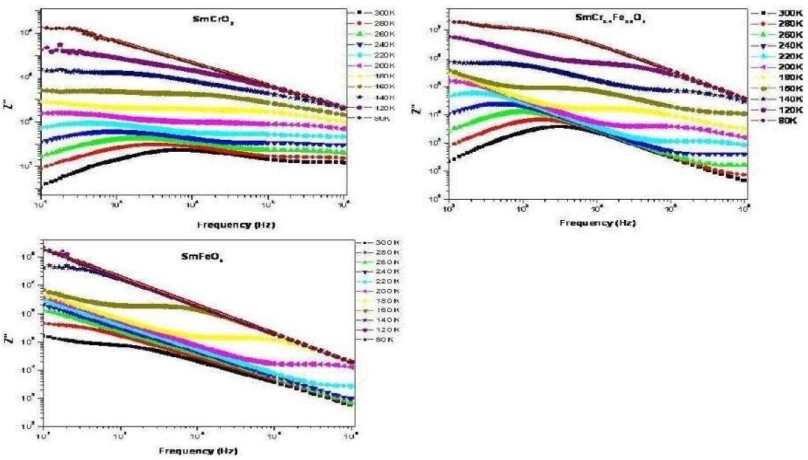

Figure 6. Plot between Z'' vs Frequency at different temperatures for $SmCr_{1-x}Fe_xO_3$ (x= 0, 0.4, 0.6, 1) ceramics.

seen. The figure 6 shows Z'' vs frequency plots for different temperatures. Inspection of these plots over the measured temperature range revealed the presence of a peak which is shifting from low to high frequency with increase in temperature. For temperatures above 200K the peak is moving out of measuring window is corresponds to bulk (grain) and at low frequencies for temperatures above 180K we can observe another peak which is shifting from low to high frequencies is correspond to grain

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boundary.

4. Conclusion

Ceramic samples of $SmCr_{1-x}Fe_xO_3$ (x= 0, 0.4, 0.6, 1) ceramics characterized using XRD and SEM. With increase in Fe content porosity is decreasing. The effective dielectric constant obtained in frequency range 100Hz to 1MHz exhibited giant dielectric constant value ~10^4 at room temperature. dielectric constant ε' (T) features a step like transition at temperatures ranging from 100 K (< 100 kHz) to 280 K (1MHz). This step like transition was linked with thermally activated dielectric relaxations. With increasing Fe content grain boundary response is decreasing. The observed temperature and frequency dependent high dielectric constant in semiconducting SCFO ceramics is dominated by gain boundary response.

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