Structural and electrical characterization of $SrCeO_3$ and Sr_2CeO_4

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Abstract: Extensive research has been carried out on $SrCeO_3$, reported as potential candidate for solid electrolyte of intermediate temperature solid oxide fuel cells [1]. Strong emission exhibited by rare-earth doped Sr_2CeO_4 in visible range makes it a potential candidate for applications in field emission displays (FEDs) [2]. Sr_2CeO_4 is a compound closely related to perovskite compound $SrCeO_3$ is composed of SrO layers separating by $SrCeO_3$ block layers. Electrical properties of $SrCeO_3$ as well as optical properties of Sr_2CeO_4 have been well studied. Hence, to explore more applications the electrical properties of Sr_2CeO_4 have been studied and compared with electrical properties of $SrCeO_3$,is considered worthwhile. Therefore, in this work synthesis of the $SrCeO_3$ and Sr_2CeO_4 has been carried via conventional solid state reaction route using high purity (≥ 99 %) raw materials $SrCO_3$ and cerium ammonium nitrate $(NH_4)_2Ce(NO_3)_6$. Thermal analysis (TGA/DSC) of the mixture of raw materials prepared for both the compounds illustrated that the decomposition of cerium ammonium nitrate $(NH_4)_2Ce(NO_3)_6$ into CeO_2 occurs in the temperature RT-200 ^oC whereas of $SrCO_3$ into SrO above 800^{o}C.Thermal analysis (TGA-DSC) of a stoichiometric mixture of raw materials $SrCO_3$and CeO_2 for $SrCeO_3$ (1 mole : 1 mole) and Sr_2CeO_4 (2 mole : 1 mole) has been carried out up to 1000 ^{o}C with a heating rate of 10 ^{o}C/min in N_2 gas atmosphere were recorded. TGA-DSC curves areshown in Figure 1 (a) and 1(b) respectively for $SrCeO_3$ and Sr_2CeO_4. The TGA curves show total weight loss approximately 13.48 % and 20.41 % accompanied by an endothermic peak in DSC curves at 900^{o}C and 950^{o}C for $SrCeO_3$ and Sr_2CeO_4, respectively. The endothermic peak is attributed to the reaction between raw materials to form desired phase $SrCeO_3$ and Sr_2CeO_4. Based on the results of thermal analysis, mixtures of raw materials were calcined at 1000 ^{o}C for 14 h. Rietveld refinement of the XRD dada (Figure 1) confirmed that both the compounds have orthorhombic crystal structure with space group Pnma and Pbam for $SrCeO_3$ and Sr_2CeO_4, respectively. The values of lattice parameters and cell volume are presented in Table 1. The crystalline sizes (D) have been calculated for high intensity Bragg's peak corresponding to (112) and (130) reflection for $SrCeO_3$ and $Sr_2CeO_4$by using Scherer's formula and given in Table 1. The experimental density (d_{exp}) of the sintered pellets of the samples is obtained using Archimede's principle and the theoretical density (d_{th}) from their molecular weight and lattice parameters. The percentage porosity of the samples was calculated using obtain the value of experimental and theoretical density as shown in Table 1. Scanning electron micrograph (SEM) of the fracture surfaces of sintered pellets of $SrCeO_3$ and Sr_2CeO_4 shows dense structure with negligible porosity.

The average grain size of the samples was calculated using 'ImageJ' software and found to be 1.99 and 2.84 µm for $SrCeO_3$ and Sr2CeO_4 respectively.The alternating current conductivity (σ_{ac}) of synthesized samples was measured in the frequency range of 1Hz -1MHz and temperature range of 200 -600^{o}C (Figure 2). Conductivity spectra of both the samples followed universal Johnscher's power law given by;

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$$\sigma'(\vartheta) = \sigma_{dc} + A\omega^p = \sigma_{dc}[1+(\frac{\vartheta}{\vartheta_H})^p]$$

In the above equation σ_{dc} is the dc conductivity, ϑ_H is the hopping frequency (frequency at which crossover from dc to the dispersive conductivity takes place)

Fig. 1 Rietveld refinement of room temperature XRD profile.

Table 1. Structural parameters obtained from Rietveld refinement of room temperature X-ray diffraction (XRD) data.

Sample	Lattice Parameters(Å)	Cell Volume(Å)³	Crystallite Size(nm)	Experimental Density(g/cm³)	Theoretical density (g/cm³)	% Porosity
$SrCeO_3$	a=6.131 b=8.560 c=5.995	316.80	53	5.39	5.72	5.76
Sr_2CeO_4	a=6.120 b=10.349 c=3.597	227.81	47	5.22	5.42	3.69

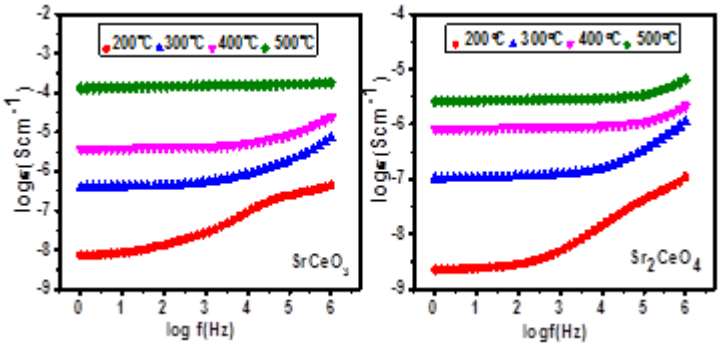

Figure 2: Variation of logarithm of ac conductivity with logarithm of frequency at few different temperatures. and p is power exponent, represents the electrical relaxation behavior of the material whose value is usually less than unity. The value of σ_{dc}dc electrical conductivity is found to be 4.20 x 10^{-6} and 3.34 x 10^{-6} S cm^{-1} for $SrCeO_3$ and Sr_2CeO_4, respectively.

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