

Structural and Optical Properties of $Y_{1-x}Sr_xCrO_3$ ($x = 0.0, 0.1$)

Pallavi Saxena^{1, a)}, A. Yadav^{1, 2, b)}, P. Choudhary¹, Meenu Dinesh Varshney¹ and A. Mishra¹

¹*Materials Science Laboratory, School of Physics, VigyanBhavan, Devi Ahilya University, Khandwa Road Campus, Indore 452001, India.*

²*Department of Physics, Medi-Caps University, Pigdamber, Indore 453331, India.*

^{a)}pallaviphy12@gmail.com

^{b)}anand.212@gmail.com

Abstract. In this paper, we have investigated the crystal structure and optical behaviour of Alkaline earth metal (Sr) doped $Y_{1-x}Sr_xCrO_3$ ($x = 0.0, 0.1$) ceramics. All the samples were synthesized successfully by ceramics solid-state reaction route. From X-ray diffraction (XRD) pattern of $Y_{1-x}Sr_xCrO_3$ ($x = 0.0, 0.1$) ceramics, we have found that there is no change in crystalline structure and it was indexed in the orthorhombic structure possessing space group $Pbnm$. FTIR spectra reveals the appearance of sharp peaks at 577, 485 and 416 cm^{-1} for pristine $YCrO_3$ and 566, 477 and 415 cm^{-1} for $Y_{0.9}Sr_{0.1}CrO_3$. These modes attributes to Cr–O stretching, Y–O stretching and O–Cr–O deformation vibration, respectively. It has been observed that 10% doping of Sr ion reduces the band gap. The band gap of $YCrO_3$ and $Y_{0.9}Sr_{0.1}CrO_3$ samples varies from 2.31 to 2.23 eV.

INTRODUCTION

We study the Sr^{2+} substitution effect on the crystal structures and optical properties of $YCrO_3$ by replacing Y^{3+} for Sr^{2+} . The focus of this study, Yttrium chromite ($YCrO_3$), is a p -type semiconductor with a perovskite structure. It is insulating in both ferromagnetic and antiferromagnetic ordered states. $YCrO_3$ crystallizes with an orthorhombic structure, with $Pbnm$ centrosymmetric space-group. $YCrO_3$ which has a ferroelectric transition temperature ~ 450 K. Recently, $YCrO_3$ has been considered as a potential multiferroic compound. It behaves as a weak ferromagnet, and below $T_N \sim 140$ K it shows a G-type magnetic arrangement. These properties make $YCrO_3$ a promising candidate for many technologically applications, such as solid oxide fuel cells, humidity sensor, in addition to the potential magnetoelectric application [1].

Alkaline earth metal were usually doped into A-site in $YCrO_3$. It has been reported that Ca doping at A-site in $YCrO_3$ reports the poor electrical conductivity, as a consequence of the formation of small-polarons. Substitution of alkaline earth metal also improves the sinter ability. Doping transition metals is seen to improve the absolute value of electrical conductivity in both oxidizing and reducing atmospheres [2].

Pure $YCrO_3$ has the perovskite structure that is apparently stable to at least 1200 K. However, its application was limited due to the relatively low electrical conductivity. There is a need to improve features of the perovskite to obtain a wider range of application. Generally, partial substitution at A-site, at B-site or both sites simultaneously, can enhance their utility by improving or changing physical and chemical properties [3]. Considering the importance of $Y_{1-x}Sr_xCrO_3$ ($x = 0.0, 0.1$) the present work reports the preparation, characterization and optical properties of Sr doped $YCrO_3$.

EXPERIMENTAL DETAILS

Polycrystalline Sr^{2+} doped $\text{Y}_{1-x}\text{Sr}_x\text{CrO}_3$ ($x = 0.0, 0.1$) samples are prepared by solid state reaction method. Y_2O_3 , Cr_2O_3 , Sr_2O_3 were used as starting material in this method. The above materials were weighed in a stoichiometric ratio and then thoroughly mixed for 6h. This mixture was calcined at a temperature of 1200°C for 14h so that the reaction takes place. The mixture was fired again at 1300°C for 14h after a grinding of 5 h. The resultant powder was pressed into circular discs of the diameter of 10mm with the thickness of 1.2 mm. The pellets were sintered for 25 hours at a temperature of 1400°C . The synthesized samples of YCrO_3 and $\text{Y}_{0.9}\text{Sr}_{0.1}\text{CrO}_3$ are further designated as YCO and YSCO, respectively.

The crystal structure of the $\text{Y}_{1-x}\text{Sr}_x\text{CrO}_3$ ($x = 0.0, 0.1$) were identified via the X-ray powder diffraction technique at room temperature using a Bruker D8-Advance X-ray diffractometer with $\text{CuK}_{\alpha 1}$ (1.5406 \AA) radiation. The data were obtained with a step size of 0.02° over the angular range ($20^\circ \leq 2\theta \leq 80^\circ$) by generating X-ray 40 kV and 40 mA power settings. Rietveld refinement was conducted on the XRD data using the Fullprof software. Fourier transform infrared (FTIR) spectra were recorded as ATR based Frontier Perkin-Elmer (SP 10 STD) in the frequency range $4000 - 400 \text{ cm}^{-1}$. UV-Vis spectrometer (Perkin Elmer, Lambda 950 - USA) was used to find the band gap of all the samples under investigation.

RESULTS AND DISCUSSIONS

The crystal structure of the samples were examined by x-ray diffraction (XRD). The XRD data was further refined through Rietveld Refinement using FullProf software [4] to confirm the phase and crystal structure of the prepared samples. The plotted Rietveld refinement of XRD pattern have been displayed in Figure 1. The analysis of XRD spectra revealed the sample crystallized in the orthorhombic structure possessing space group $Pbnm$. The slight increase in the value of lattice parameters of YSCO as compared to the pristine YCO were obtained. It can be attributed to the difference in the ionic radii of Y (0.893 \AA) and Sr (1.12 \AA) [5, 6]. The crystallite size of the samples has been calculated using classical Scherer's formula, $t = k\lambda/[\beta \cos\theta]$, where, λ is wavelength of X-ray used (1.5406 \AA), k is a constant (shape factor = 0.9), θ is the angle of diffraction, and β is the FWHM and the size of the crystallites was obtained 56nm for YCO and 61nm for YSCO. The details of the refined parameters obtained from Rietveld refinements are demonstrated in Table 1.

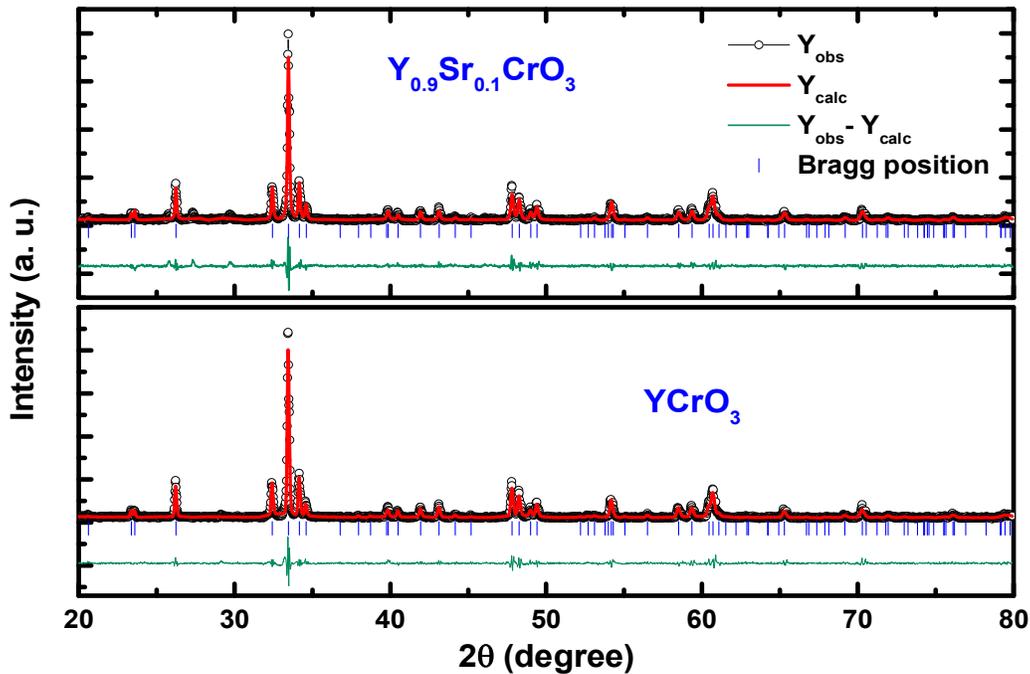


FIGURE 1 Rietveld refined XRD pattern of the $\text{Y}_{1-x}\text{Sr}_x\text{CrO}_3$ ($x = 0.0, 0.1$).

Materials	Space group	a (Å)	b (Å)	c (Å)	χ^2	GOF
YCrO_3	$Pbnm$	5.245	5.518	7.536	2.12	1.5
$\text{Y}_{0.9}\text{Sr}_{0.1}\text{CrO}_3$	$Pbnm$	5.246	5.519	7.538	2.28	1.5

To confirm the bonding in the prepared samples and hence the sample formation, we did FTIR. And the spectra obtained is displayed in **Figure 2**. It has been reported that chromium oxide generally displays the absorption bands below 1000 cm^{-1} as a result of inorganic molecular vibrations [7]. The sample formation sintered at 1400°C has been witnessed by the appearance of sharp peaks at 577 , 485 and 416 cm^{-1} for pristine YCrO_3 and 566 , 477 and 415 cm^{-1} as depicted in **Figure 2** and these peaks were attributed to Cr–O stretching, Y–O stretching and O–Cr–O deformation vibration, respectively. These absorption bands have shifted towards lower wavenumber when doped by Sr and the results are in agreement with the reports.

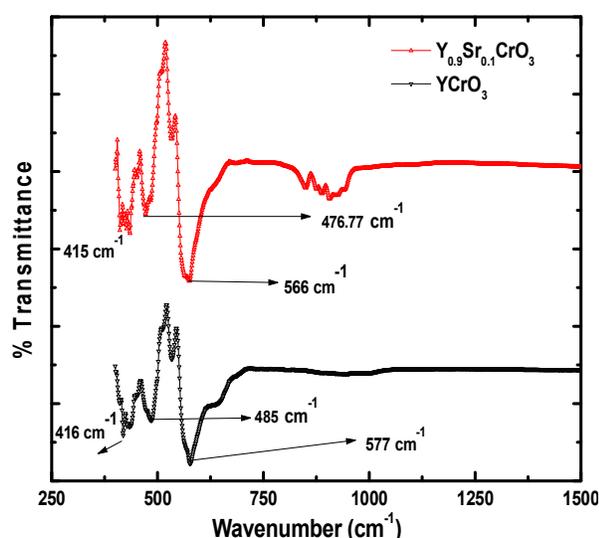


FIGURE 2 FTIR spectra of the $\text{Y}_{1-x}\text{Sr}_x\text{CrO}_3$ ($x = 0.0, 0.1$).

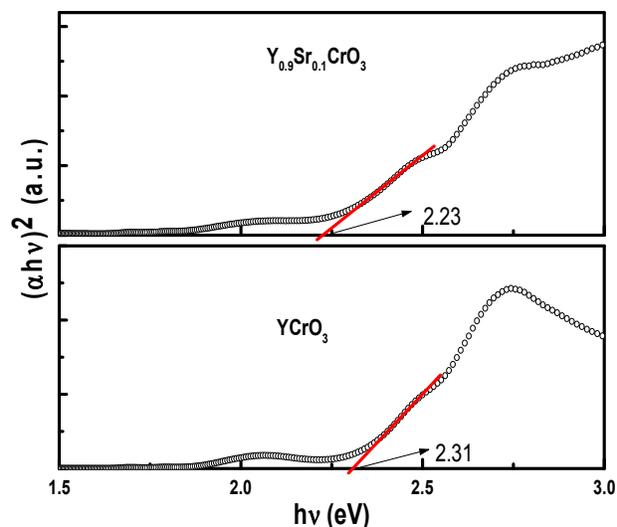


FIGURE 3 UVVIS spectra of the $\text{Y}_{1-x}\text{Sr}_x\text{CrO}_3$ ($x = 0.0, 0.1$).

The influence of alkaline earth metal (Sr) doping on the optical band gap energy of pristine YCO was investigated for which the optical diffuse reflectance spectra were recorded using UV-Vis spectroscopy. The optical band gap of the YCO and YSCO samples is calculated using Kubelka–Munk (KM) function $F(R) = (1-R)^2/2R = \alpha/s$, where R is the reflectance of the sample relative to the reference, n depends on nature of transition, α is the absorption coefficient, and s is the scattering coefficient. The band gap of the different samples is estimated by extrapolating the linear part of the graph $(\alpha hv)^2$ versus $h\nu$ (photon energy) as shown in the **Figure 3**. It has been observed that band gap decreases with the 10% Sr doping. The band gap of YCO and YSCO samples varies from 2.31 to 2.23 eV. The reduction in band gap may be due to the creation of hole carriers in the stable YCrO_3 as a result of divalent Sr^{2+} replacing trivalent Y^{3+} [1, 8].

CONCLUSIONS

In summary, $\text{Y}_{1-x}\text{Sr}_x\text{CrO}_3$ ($x = 0.0, 0.1$) samples were successfully obtained via solid state reaction method. The XRD data showed very narrow diffraction peaks indicating that samples have good crystallinity. The Rietveld refinement reveals that all samples belong to the orthorhombic structure with space group $Pbnm$. The FTIR spectra of YCO shows sharp peaks at 577 , 485 and 416 cm^{-1} and 566 , 477 and 415 cm^{-1} and for YSCO. These peaks were attributed to Cr–O stretching, Y–O stretching and O–Cr–O deformation vibration, respectively. The optical band

gaps of the YCO and YSCO samples were determined. The YCO manifested by a sharp band gap at 2.31 eV. On the other hand, YSCO shows reduced band gap at 2.23 eV.

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