International Journal of Science and Research (IJSR)
ISSN (Online): 2319-7064
Index Copernicus Value (2013): 6.14 | Impact Factor (2013): 4.438

Physical and Structural Characterization of Chromium Ions Doped SrO-Li_2O-CaO-B_2O_3 (SLCB) Glasses

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Abstract: ***The physical and structural characterization of Chromium ions doped xSrO–(20-x) Li_2O–(10-y) CaO-70B_2O_3-y, (x=5, 10, 15 mol %) and y=0.1mol %(Cr_2O_3) (SLCB) glasses have been studied. Choices of physical parameters are evaluated for the synthesized glasses. The X-ray diffractograms (XRD) of all the synthesized glass samples confirm the non crystalline character. The Fourier Transform-Infrared (FT-IR) spectral investigations of chromium ions doped glasses exhibits characteristic vibrations of BO_3 units.***

Keywords: XRD, FT-IR.

1. Introduction

Glasses are amorphous materials and are transparent in the visible region. The structure of oxide glasses reveal their ionic conductivity and potential usage as solid electrolytes in a variety of electrochemical devices like solid state batteries, fuel cells, chemical sensor and smart windows [1]. Among all the classical network formers, boric oxide (B_2O_3) is one of the significant glass former and flux material due to their high phonon energies [2]. Borate glasses have special features such as high thermal stability and good solubility, making them promising candidates for a vast amount of technological applications [3, 4]. The strontium oxide has also been extensively used as a component ensuring an improvement of a number of physiochemical properties of glasses [5]. The simplest physical property of any solid that can be measured easily is density. It is a highly informative property if the structure of the material could be well defined. Density data is used to calculate the volumes of structural units.

2. Experimental

2.1 Glass preparation

A Series of chromium ions doped SLCB glasses are prepared by using analar grade (AR) chemicals, $SrCO_3$, Li_2CO_3, CaO, H_3BO_3 and Cr_2O_3 as starting materials with 99.9% purity. The compositions of all the glass samples are given in **Table 1.**

Table 1

Batches with xSrO-(20-x)Li_2O-(10-y) CaO-70B_2O_3-y, Cr_2O_3 compositions for glass making and their corresponding codes.

Glass System	Glass Code	Glass chemical Composition
SLCB 0	Cr 0	10 SrO+10 Li_2O+10 CaO+70 B_2O_3+ ---
SLCB 1	Cr 1	5 SrO+15 Li_2O+9.9 CaO+70 B_2O_3 +0.1 Cr_2O_3
SLCB 2	Cr 2	10 SrO+10 Li_2O+9.9 CaO+70 B_2O_3 +0.1 Cr_2O_3
SLCB 3	Cr 3	15 SrO+5 Li_2O+9.9 CaO+70 B_2O_3 +0.1 Cr_2O_3

For the preparation of about 10 g of each batch, appropriate amounts in wt. % of chemicals in powder form are taken mixed thoroughly in mortar and pestle. The batches are transferred to porcelain crucibles and kept in an electrical furnace for a time of 20 min. maintained at a temperature of 1223K. The melts are poured on the surface of a plane brass plate and pressed quickly with another brass plate. The thin glasses formed are annealed for about 1 hr to relieve from mechanical stress. Transparent and greenish colored glasses are obtained

2.2 Measurements

The density 'ρ' of glass samples are determined from the Archimedes's principle by using xylene as an inert buoyant liquid and some other physical parameters are evaluated. The powder X-ray diffractograms of prepared glass samples are recorded using copper target Kα radiation by 6100 (Shimadzu) diffractometer at room temperature. The infrared spectra of the powdered glass samples are recorded using IR Affinity-1s (Shimadzu) infrared spectrometer in the wave number range of 400-4000 cm^{-1} at room temperature with KBr pellet technique.

3. Results and Discussion

3.1 Physical parameters

Using the measured glass density 'ρ', values, various physical parameters i.e. average molecular weight (M), chromium ion concentration (N_i), mean chromium ion separation (r_i) and the polaron radius (r_p) are evaluated using conventional formulae given in previously reported literature [6]. It is observed that the density is minimum for 5% SrO, 15% Li_2O and maximum for 15% SrO, 5% Li_2O glasses. The density value of the undoped glass and the glass doped with 0.1 mol% of Chromium ions and 10% SrO, 10% Li_2O are nearly equal. The values obtained are given in **Table 2.**

3.1.1 Optical basicity

The optical basicity of an oxide glasses can be conveniently measured in terms of the ability of the glass to donate a negative charge to an acidic probe ion [7-10]. Duffer and Ingram [11] reported that the optical basicity can be predicted from the composition of the glass and the basicity moderating parameters of various cations present. The theoretical values of optical basicity (Λ_{th}) of glasses can be estimated using the formula,

$$(\Lambda_{th}) = \sum_{i=1}^{n} \frac{Zi\,ri}{2\gamma i} \quad (1)$$

where 'n' is the total number of cations present. Z_i is the oxidation number of the i^{th} cation to the number of oxides present and 'γ_i' is the basicity moderating parameter of the i^{th} cation. The basicity moderating parameter 'γ_i' can be calculated from the following equation

$$\gamma_i = 1.36(x_i - 0.26) \quad (2)$$

where x_i is the Pauling electro negativity of the cation [12]. The theoretical optical basicity values computed of the glasses in the present study are given in **Table.2**.

Table 2
Physical parameters of Chromium ions doped in SLCB glasses.

Physical Parameters (Units)	Glass System			
	$SLCB_0$	$SLCB_1$	$SLCB_2$	$SLCB_3$
Average molecular weight(M)(g/mol)	67.69	64.04	67.73	71.42
Density (gr/cc)	2.65	2.54	2.64	2.77
Transition metal ion (N_i) Concentration (10^{+19}ions/cc) (±0.005)	…..	2.38	2.36	2.34
Inter ionic distance (r_i)(A^0)(±0.005)	…..	34.71	34.90	34.94
Polaron radius (r_p)(A^0)(±0.005)	…..	13.98	14.06	14.05
Optical basicity (Λ_{th})	0.43	0.43	0.43	0.42

It is observed that the Λ_{th} values gradually increases from $SLCB_1$ to $SLCB_3$. It is observed that the optical basicity value is minimum for a glass with 15% SrO, 5% Li_2O and maximum for 10% SrO, 10% Li_2O contents.

3.2 Powder XRD

The powder XRD diffractograms of undoped and chromium ions doped glasses are shown in **Fig.1.** This reveals the amorphous nature the synthesized glasses.

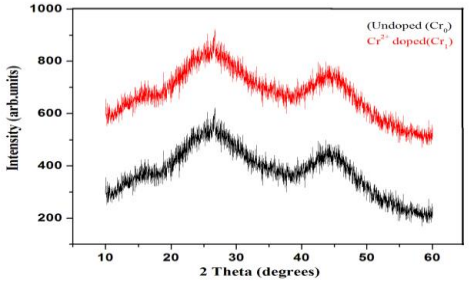

Figure 1: X-ray diffractograms of undoped and Chromium ions doped SLCB glasses.

3.3 FT-IR Studies

The IR spectra of SLCB glasses are shown in **Fig.2**.

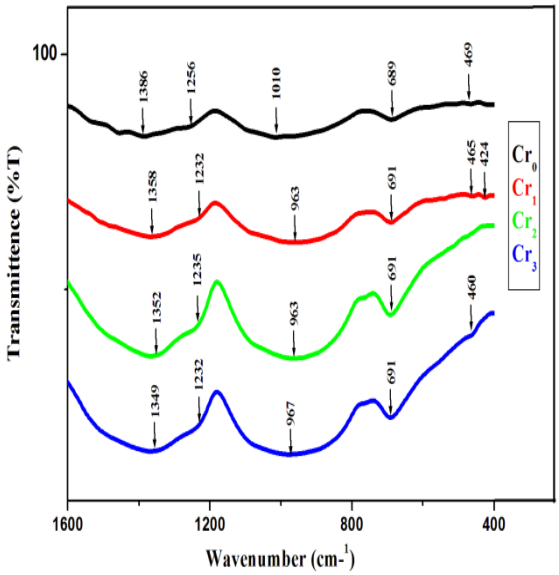

Figure 2: FT-IR spectrum of Cr^{3+} ions doped SLCB glasses.

The assignments of various bands are given in **Table 3**.
The IR spectra can be alienated into three regions such as 600–800 cm^{-1} which are due to B-O-B bending vibrations of various borate units. The second region 800 – 1200 cm^{-1} is attributed to B-O symmetric vibrations of tetrahedral BO_4 units. The third region 1200–1600 cm^{-1} is related to B-O stretching vibrations of BO_3 units [13-15]. The spectra contain three broad and intense absorption bands centered around 1386 cm^{-1}, 1010 cm^{-1} and 686 cm^{-1}, with some shoulders and feeble bands are also observed in the undoped (Cr_0) sample. The broad band around 1386 cm^{-1} and the and the shoulder around 1256 cm^{-1} are due to symmetric stretching vibrations of B-O bonds in BO_3 units varied from types of pyro, ortho borate groups respectively. The intensity of the broad band and the shoulder increases with the increase of SrO content. The broad band around 1010 cm^{-1} is due to boroxil rings [16]. This band is the characteristic of glass containing high B_2O_3 content. The intensity has increased with the increase of SrO content. The absorption band at 689 cm^{-1} is due to B- O-B deformation vibrational mode [17, 18]. The intensity of the band increases with increase in SrO content. The shoulder at 469 cm^{-1} is due to Ca-O_6 stretching mode of Borate units.

Table 3
Assignment of the bands in the infrared spectra of Chromium ions doped in SLCB glasses.

Cr_0	Cr_1	Cr_2	Cr_3	Assignment
-	424	-	-	Ca-O stretching mode of BO_3 units
469	465	-	460	Ca-O_6 stretching mode of BO_3 units
689	691	691	691	B-O-B bending
1010	963	963	987	B-O stretching Vibrations
1256	1232	1235	1232	Stretching vibrations B-O

				bonds in BO_3 Units from pyro-ortho borate groups
1386	1358	1352	1349	Stretching vibrations of B (III)-O-B (IV)- units

The intensity at this peak is maximum for 15 mol% of SrO and 5 mol% of Li_2O [19].

4. Conclusion

1) The density values are increasing with the increase of SrO mol%.
2) The optical basicity value is maximum when the mol% of SrO and Li_2O are equal i.e. 10%.
3) XRD has confirmed the amorphous nature of the
4) Present glasses under study.
5) The FT-IR spectra have shown the characteristic

Spectra of Borate glasses.

5. Acknowledgements

One of the authors **M. Ratna Raju**, F.No.APNA071, FDP/FIP-XI Plan is thankful to the UGC-SERO, Hyderabad, for providing financial assistance under FDP Program to carry out this work.

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