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Structural Characterization of fly ash doped lithium borate Glasses

JARNAIL SINGH[1], GURMELSINGH[1],NEETU CHOPRA[2],GAGANDEEP SINGH[3], and GOPI SHARMA[2]

[1] *Department of Physics, Punjabi University, Patiala.*
[2] *Department of Physics, Kanya Maha Vidyalaya, Jalandhar, Punjab, India.*
[3] *Department of Chemistry, Lyallpur Khalsa College, Jalandhar, Punjab, India.*
Tel: +919888014241 E-mail: sharmagopi28@yahoo.com,

Lithium borate glasses with fixed alkali content of 10 Mole % and different modifiers have been prepared. To compare the role of fly ash as a glass modifier the content of glass modifier PbO, Al2O3 have been kept same to 5 mole %. To investigate the structure FTIR and UV-VIS spectra of prepared samples have been taken. From optical data optical band gap and cutoff wavelength have been calculated. Density of prepared samples has been calculated by using Archimedes principle. Results have been compared with structure of binary lithium borate glass. This work can lead to future application of utilization and characterization of fly ash in glass forming materials.

Key Words: Fly ash, Optical band gap. Glass modifier

INTRODUCTION

Structural characterization of borate glasses have always been an interesting subject due to numerous applications of borate glasses in technology. Borate glasses are characterized by complex dependences of the properties on the composition. The structural interpretation of these dependences in different works is very contradictory and does not always agree with experimental data. The most widely accepted model for structure of vitreous B_2O_3 is random network of corner linked BO_3 triangles as suggested by Zachariasen [1]. The triangular BO_3 structural units are deduced from the boron-oxygen configuration in crystalline borates. Although boron occurs in both triangular and tetrahedral coordination in crystalline compounds, it is believed to occur only in triangular state in vitreous boric oxide. The structure of vitreous boric oxide is also believed to contain a large concentration of unit consisting of three boron-oxygen triangles joined to form boroxol ring structure [2].

The introduction of oxygen from a modifier oxide to boric oxide glass can create structural changes and hence properties of glass matrix. It is therefore interesting to visualize the effect of different modifiers on structure of borate glasses. Recently [3-8] glasses with fly ash have been center of investigation due to environmental concern for consumption of fly ash.

Therefore the main objective of the present work is to study structural changes induced by different modifiers on optical and physical properties of lithium borate glasses and to compare the structural changes induced by fly ash in borate network.

EXPRIMENTAL TECHNIQUES

Glass making: Glass samples of the type $0.10Li_2O$–$0.90 B_2O_3$ (sample no. L_1), $0.1Li_2O+0.85B_2O_3+0.05Al_2O_3$ (sample no. L_2), $0.10 Li_2O$–$0.85 B_2O_3$–$0.05PbO$ (sample no. L_3), $0.10 Li_2O$–$0.85 B_2O_3$–0.05 Flyash (sample no. L_4) were prepared by using the melt–quenching technique. Commercial grade chemicals of Li_2O and B_2O_3 (Aldrich Chemical Company) were used as starting materials. Fly ash used in present work was obtained from National Fertilizers Limited, Bathinda, India. Appropriate amounts of oxides were weighed by using an electronic balance having an accuracy of 0.001 g. The chemical compositions of all these glasses are shown in Table 1. The chemicals were then mixed in a pestle mortar for half an hour. The crucible containing the batch was heated in an electric furnace at a temperature of 900 ºC for half an hour under normal atmospheric conditions and then dry oxygen was bubbled through it using a quartz tube to ensure homogeneity of the glass melt. Heating was performed for a longer period of time. The melt was then poured into a graphite mould. The glass samples were then annealed in a separate annealing furnace for twelve hours. The samples were grounded with the help of an electric machine using different grades of SiC abrasives and aluminium oxide with machine oil by setting the sample in a specially designed holder to maintain the two faces parallel. The polishing was done with cerium oxide to obtain flatness. Thickness measurement was carried out by micrometer.

Table 1: Composition Mole fraction of glass samples

Sample No.	Li_2O	B_2O_3	Al_2O_3	PbO	Fly ash
L_1	0.10	0.90	–	–	–
L_2	0.10	0.85	0.05	–	–
L_3	0.10	0.85	–	0.05	–
L_4	0.10	0.85	_	–	0.05

Optical measurements: The optical measurements were made using a UV-VIS spectrometer (Shimadzu, Japan), together with a dual light source capable of outputting ultraviolet as well as visible light. Working in the wavelength range of 200 – 900 nm, percentage transmission spectra was calculated using air as the reference and optical cut off was obtained by finding the intercept of the steepest slope of the rapid transmission drop–off with the baseline preceding it.

Infrared absorption spectra of powdered glass samples were measured in the range of 400–4000 cm^{-1} using KBr technique at room temperature. A recording spectrometer of type Perkin Elmer–1600 was used. Infrared spectra were corrected for the dark current noise and background using a two point baseline correction. The spectra were normalized by making absorption of any spectrum varies from zero to one arbitrary units. The *density* was obtained from Archimedes' principle using benzene as buoyant.

RESULTS AND DISCUSSION

Density: The measured values of density for present glass composition are lists in Table 2. It has been found that density increases linearly from L_1 to L_3. This indicates that with addition of 5 mole % of modifier in lithium borate glass composition a compact structure is formed and hence increase in density is observed. Where as for sample L_4 (with 5 mole % of fly ash) a decrease in density is observed. This decrease indicates that with addition of fly as a open structure is formed and hence density decreases. The major contents of fly ash used in present study is Silica so decrease in density indicates that addition of silica to borate glass makes an open configuration.

Table 2: Optical and physical data of Lithium borate glasses doped with fly ash and lead oxide.

Sample No.	Thickness cm	Density g/cm^3	Optical Band Gap eV
L_1	0.775	2.04	3.13
L_2	0.643	2.05	3.11
L_3	0.637	2.45	3.09
L_4	0.902	2.06	2.57

Fourier transform Infrared studies: In the present work Fig. 1 shows the spectra of L_1, L_2, L_3, L_4 glasses. For L_1 sample the main band is located at 689, 1050, 1400 cm-1. Upon aluminium addition some new bands are seen at 710, 506, 984 cm-1. For L_4 sample the position of bands is near to L_2 sample. Where as for L_3 sample a very clear but broad band is observed at around 1000 cm-1. A broad band for L_4 sample at 1432 cm-1 indicates increase in non bridging oxygen ions (NBOs) with addition of fly ash. Similarity of L_2 and L_4 samples can be attributed to contribution of aluminium from fly ash. The present findings are in line with the investigation of previous workers [9-13].

Optical band gap: Optical band gap has been calculated by model proposed by Mott and Davis [14]. According to this model, the absorption coefficient α varies with the angular frequency ω in the following manner:

$$\hbar\omega\alpha(\omega) = B\left[\hbar\omega - E_0\right]^2 \qquad (1)$$

Where B is a constant. In order to calculate the mobility gap (E_0), a graph was plotted between $[\hbar\omega\alpha(\omega)]^{1/2}$ and $\hbar\omega$ for each sample and from the linear extrapolation to zero ordinate, the value of E_0 was calculated (Fig. 2). Table 3 lists the calculated values of optical band gap. A decrease in band gap has been found from samples L_1 to L_4. This is in agreement with density measurements and further indicates that a compact state is formed from glass samples L_1 to L_3 and hence decrease in band gap is observed. For glass sample with 5 mole % fly ash content (L_4) this decrease in band gap can be attributed increase in non bringing oxygen with addition of silica.

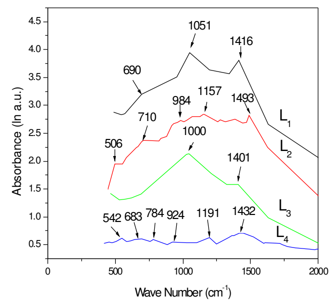

Fig. 1. FTIR spectrum of L_1, L_2, L_3 and L_4 glasses

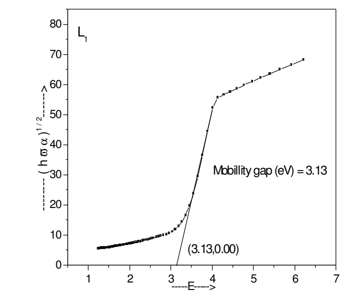

Fig. 2 Optical Band gap for sample L_1

Conclusion

Addition of fly ash plays a role as a glass modifier similar to role played by PbO and Al_2O_3. Increase in non bridging oxygen ions is observed with fly ash addition and hence decrease in density and band gap is observed. Further attempt can also be made to increase the fly ash content to elucidate its role from glass modifier to former.

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