

Full Length Research Paper

Infrared Spectra and Energy band gap of Potassium Lithium Borate glass dosimetry

Haydar Aboud*, H. Wagiran, I. Hossain and R. Hussin

Department of Physics, Universiti Teknologi Malaysia, Skudai 81310, Malaysia.

Accepted 26 January, 2012

Fourier transform infra red (FTIR) and energy band gap of potassium lithium borate glasses of different composition have been studied using Fourier FTIR and UV-VIS spectroscopy techniques. The glasses were melted in the alumina crucible in an electric furnace at 1100°C for 30 min until homogenous melt was obtained. The X-ray diffraction analysis was adopted for confirming the amorphous nature of glass samples. From optical data direct, indirect energy band gap and cutoff wavelength has been calculated.

Key words: Energy band gap, Fourier transform infra red (FTIR), X-ray diffraction, UV-VIS spectroscopy, amorphous.

INTRODUCTION

Glasses are featured by the absence of long range order in their structure. The class of solid materials is commonly termed amorphous, in contrast with the crystalline class of materials. Thus, the variations of their physical-chemical properties are also dependent on composition, processing and thermal history. Glasses have attained an ever increasing importance in materials science and technology, such as communicating sounds, visual signals, fiberglass and ceramics. Nowadays, borate is one of the significant glasses forming oxides and has been incorporated into several kinds of glass systems to attain the desired chemical and physical properties. Although, it can form a better borate glass if it was added with modifier metal oxides (Meera et al., 1990). In other words, the metal oxides act as a modifier which will change the glass structure. For instance, LiB_3O_5 (Lin et al., 2006), $\text{MgO-Al}_2\text{O}_3\text{-B}_2\text{O}_3$ (Kafadar et al., 2008) and $\text{MgB}_5\text{O}_{10}$ (Raju et al., 2009). The aim of this present work is to study the influence of the glass composition on energy band gap and the infrared (IR) spectra of the glasses under investigation.

MATERIALS AND METHODS

Preparation of the glass samples

The composition (90-x) $\text{H}_3\text{BO}_3\text{-}10\text{K}_2\text{CO}_3\text{-xLi}_2\text{CO}_3$ with x = 10, 15,

20, 25 and 30% mol of glass samples has been prepared by the melt quenching technique. The raw materials for the glass preparation were commercially obtained in powder form. The H_3BO_3 (purity 99.9%), Li_2CO_3 (purity 99.997%) and K_2CO_3 (purity 99.9%) were from Sigma-Aldrich (Germany). Required quantities of H_3BO_3 , Li_2CO_3 and K_2CO_3 were mixed together by grinding the mechanical mixture for about 40 min repeatedly to obtain a fine powder. The mixture was melted in an alumina crucible using electrically heated furnace under temperature of 1100°C for 30 min to homogenize the melt. The obtained glass samples from the melt quenching into a preheated stainless-steel mould was heat treated at a temperature of 400°C below their calorimetric glass transition temperature for 3 h to remove any internal stresses, and also subsequently cooled down to room temperature. The vitreous state was determined by X-ray diffraction (XRD) analysis to confirm that the sample is amorphous. The XRD machine was operated at 30 mA, 40 kV and the jig holding the specimen and spun at 15 rpm for uniform scanning. The scanning was between 2θ values of 10 to 70° with a step time of 5 s per step and a resolution of 0.01°.

Optical measurements

The infrared absorption spectra of the glasses in the wave number range of 200 to 2000 cm^{-1} were measured at room temperature by an infrared spectrophotometer (Perkin Elmer, Japan). The spectrum of each sample represents an average of 16 scans. The spectrum has been carried out for each sample several times to avoid errors during the measurements.

The measurement of optical absorption and the absorption edge using the UV-Vis-NIR scanning spectrophotometer for all glasses ranging from 200 to 800 nm wavelength. It is important in the study of the electronic structure of amorphous materials and for calculation of energy band gap.

*Corresponding author. E-mail: han55608@yahoo.com

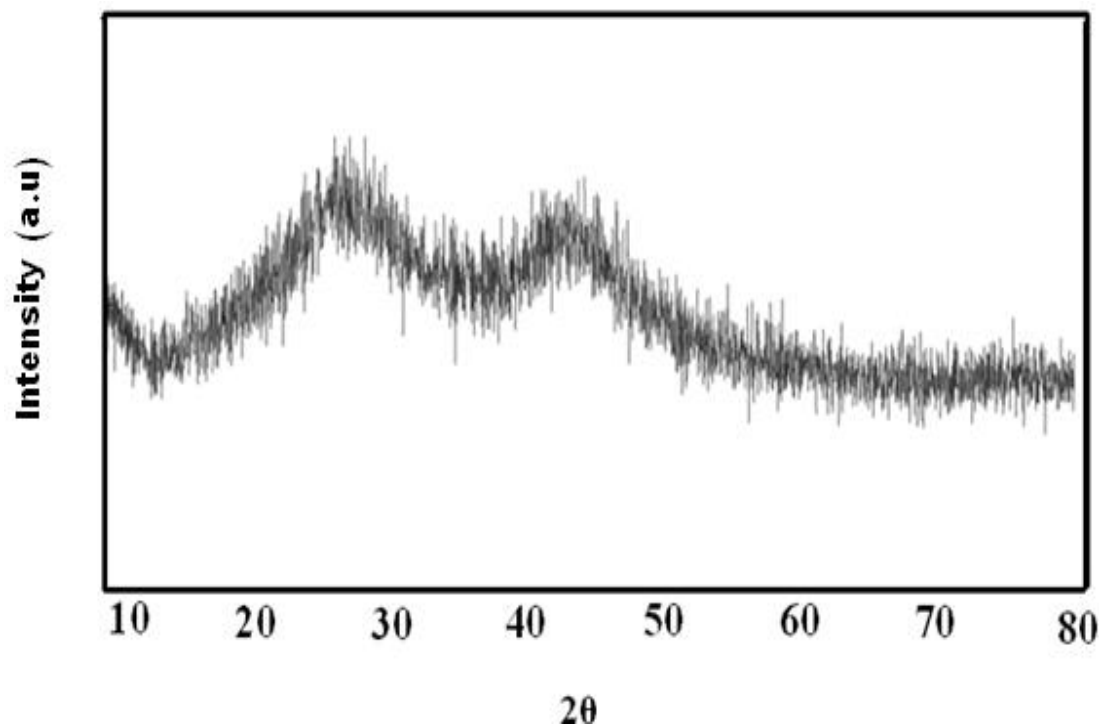


Figure 1. XRD patterns at room temperature for 80H₂BO₃-10Li₂CO₃-10K₂CO₃ glass system.

RESULTS AND DISCUSSION

X-Ray diffraction analysis

The prepared glass samples were measured by means of X-ray diffraction to confirm the amorphous state of the samples. The obtained XRD diffraction patterns are as shown in Figure 1. This confirms that the prepared samples are completely amorphous, and they do not present any crystalline phase.

FTIR spectroscopy

In general, IR analysis of absorption of the borate glasses is very high in the region of interest of wave numbers < 2000 cm⁻¹. The vibrational modes of the borate network are mainly active in three infrared spectral regions: 1200 to 1500 cm⁻¹ (B-O stretching of trigonal BO₃⁻ units), 800 to 1200 cm⁻¹ (B-O stretching of tetrahedral BO₄⁻ units) and 600 to 800 cm⁻¹ (bending vibrations of various borate segments) (Silim and Solids, 2006; Kamitsos et al., 1990). Where Table 1 and Figure 2 show characterization of borate.

Energy band gap

The band-gap energy (E_g) was determined based on numerical derivative of the optical absorption coefficient.

The fundamental absorption method refers to band to band transitions by using Mott and Davis relation of Equation 1 (Mott et al., 1971). For photon energies $h\nu$ just above fundamental edge, the absorption coefficient α follows the standard relation.

$$\alpha = (h\nu - E_g)^n A/h\nu \quad (1)$$

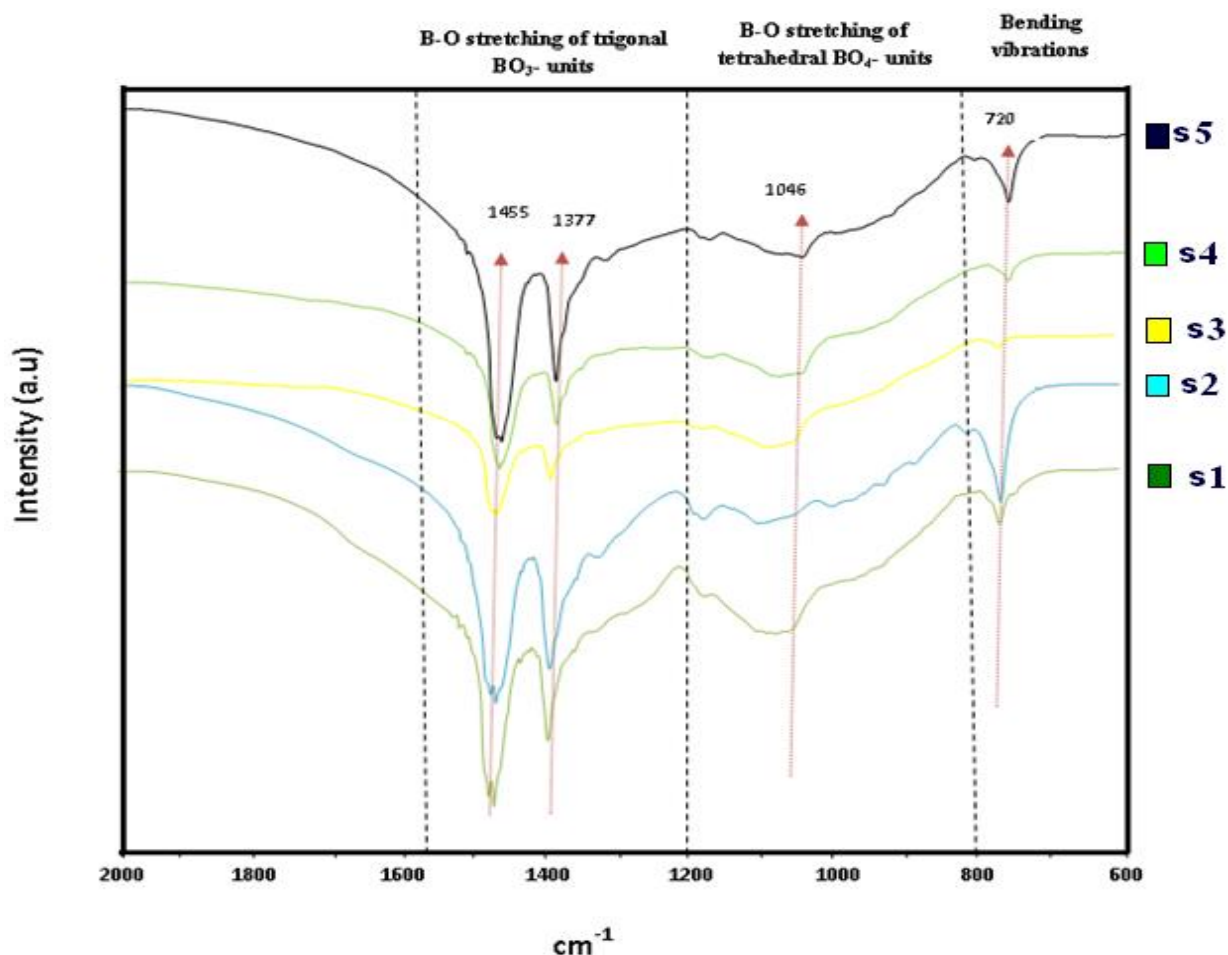
where A is a constant related to the extent of the band tailing, $n = 1/2$ for allowed direct transition, $n = 2$ for allowed indirect transition and E_g is the energy gap between the valence band and the conduction band.

A graph of $(\alpha h\nu)^2$ versus $h\nu$ is as shown in Figure 3 by extrapolating the optical band gap for all glasses. It is clear that the E_g decreasing from 3.55 to 3.40 as the amount of Li₂CO₃ increase from 10 to 30%. Figure 4 Displays the value of E_g for indirect transition for all glasses are obtained as a plot of $(\alpha h\nu)^{1/2}$ versus $h\nu$. In addition, it explained decline energy band gap from 3.52 to 3.38 as quantity Li₂CO₃ rise.

The energy gap for all samples is summarized in Table 2. It reveals the compared values for different Li₂CO₃ modifier's content. According to that, the behavior of the energy band gaps shows a gradual decrease with an increase in modifier concentration.

Table 1. The FTIR peaks positions of the $(90-x)\text{H}_2\text{BO}_3-x\text{Li}_2\text{CO}_3-10\text{K}_2\text{CO}_3$ glasses system.

| Sample number | Composition (mol%) | | | Absorption peak (cm^{-1}) | | |
|---------------|-------------------------|--------------------------|-------------------------|--|---|--------------------|
| | H_3BO_3 | Li_2CO_3 | K_2CO_3 | B-O stretching of trigonal BO_3^- units | B-O stretching of tetrahedral BO_4^- units | Bending vibrations |
| S1 | 80 | 10 | 10 | 1455-1377 | 1046 | 720 |
| S2 | 75 | 15 | 10 | 1455-1377 | 1046 | 720 |
| S3 | 70 | 20 | 10 | 1455-1377 | 1046 | 722 |
| S4 | 65 | 25 | 10 | 1458-1376 | 1045 | 722 |
| S5 | 60 | 30 | 10 | 1455-1376 | 1045 | 720 |

**Figure 2.** Infrared transmission spectra $(90-x)\text{H}_2\text{BO}_3-x\text{Li}_2\text{CO}_3-10\text{K}_2\text{CO}_3$ glasses at various compositions.

Conclusions

The glasses of composition $(90-x)\text{H}_2\text{BO}_3-x\text{Li}_2\text{CO}_3-10\text{K}_2\text{CO}_3$ system ($x = 10, 15, 20, 25$ and 30% mol), have successfully been made by melt quenching technique. The X-ray diffraction measurements have shown no existing peaks, which suggest that the glasses are in amorphous state. The FTIR spectra of alkaline for different percentage (Li_2CO_3) glasses have been found with equal number of

peaks at approximately the same wave-numbers, that is, in the regions of 600 to 800 (bending vibrations of various borate segments), 800 to 1200 (B-O stretching of tetrahedral BO_4^- units) and 1200 to 1500 (B-O stretching of trigonal BO_3^- units). The values of optical direct and indirect energy band gap decrease with an increase of modifier concentration. Moreover, the direct and indirect energy band gap decrease from 3.55 to 3.40 and 3.52 to 3.38 with decrease of boric acid.

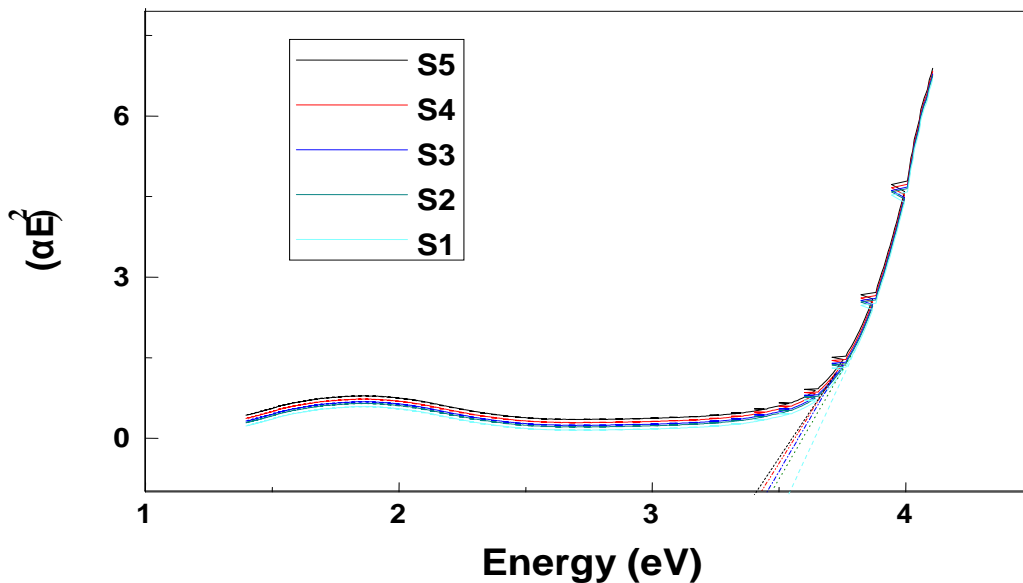


Figure 3. A graph of $(\alpha E)^2$ versus (E) for all glasses systems, direct.

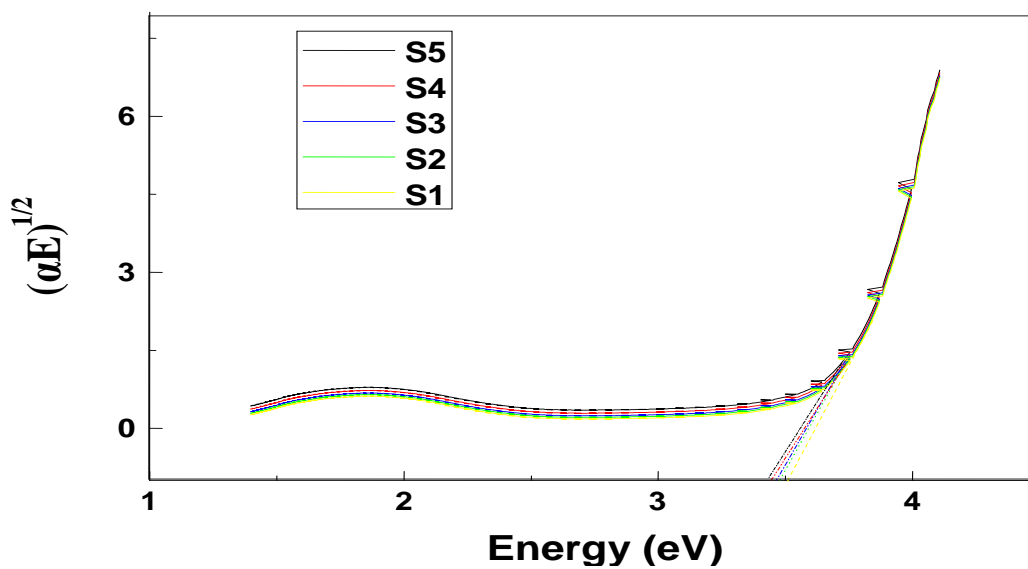


Figure 4. A graph of $(\alpha E)^{1/2}$ versus (E) for all glasses systems, indirect.

Table 2. Energy band gap of the $(90-x) \text{H}_3\text{BO}_3 - x\text{Li}_2\text{CO}_3 - 10\text{K}_2\text{CO}_3$ glasses.

| Number of sample | Composition (mol%) | | | (E_g) eV for direct | (E_g) eV for indirect | Cut-off λ nm |
|------------------|-------------------------|--------------------------|-------------------------|-----------------------|-------------------------|----------------------|
| | H_3BO_3 | Li_2CO_3 | K_2CO_3 | | | |
| S1 | 80 | 10 | 10 | 3.55 | 3.52 | 350 |
| S2 | 75 | 15 | 10 | 3.49 | 3.45 | 355 |
| S3 | 70 | 20 | 10 | 3.47 | 3.42 | 358 |
| S4 | 65 | 25 | 10 | 3.45 | 3.40 | 360 |
| S5 | 60 | 30 | 10 | 3.40 | 3.38 | 365 |

ACKNOWLEDGEMENTS

The authors are grateful for the Fundamental Research to the Universiti Teknologi Malaysia for a research studentship.

REFERENCES

- Kafadar VE, Necmeddin A, Yazici Yildirim RGu (2008). Determination of trapping parameters of dosimetric thermoluminescent glow peak of lithium triborate (LiB_3O_5) activated by aluminum. *J. Luminesci.*, 129(7): 710-714.
- Kamitsos EI, Karakassides MA, Chryssikos GD (1990). Infra-red reflectance spectra of lithium borate glasses. *J. Non-Cryst. Solids*, 126: 52-67.
- Lin CK, Yu M, Pang ML, Lin J (2006). Photoluminescent properties of sol-gel derived $(\text{La,Gd})\text{MgB}_5\text{O}_{10}:\text{Ce}^{3+}/\text{Tb}^{3+}$ nanocrystalline thin films. *Optical Material*, 28: 913-918.
- Meera BN, Sood AK, Chandrabhas N, Ramakrishna J (1990). Raman study of lead borate glasses. *J. Non-Cryst. Solids*, 126: 224-230.

- Raju GN, Ch N, Ramesh NP, Krishna TL, Srinivasulu K, Sudhkar KSV, Venkateswara RP (2009). Spectroscopic and dielectric properties of titanium doped $\text{MgO-Al}_2\text{O}_3\text{-B}_2\text{O}_3$ glass system. *IOP Conf. Series: Materials Sci. Eng.*, 2: 012031.
- Silim H, Solids A (2006). Composition effect on some physical properties and FTIP Spectra of Alumino-Borate glasses Containing Lithium, Sodium, Potassium and Barium Oxides. *Egypt, J. Solids*, 29(2): 293-302.