Optical Band Gap of glass - Various Techniques

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Abstract- Optical absorption spectra for mixed alkali borosilicate glass was obtained by UV-Vis Spectroscopy and energy gaps are calculated using Tauc Plots and also from Diffuse Reflectance spectra using Kubelka -Munk function. Bandgap is also calculated from first derivative of absorption spectra and all the values of band gaps obtained from various methods are compared.
Index terms: mixed alkali borosilicate glass, UV-Vis Spectroscopy, Bandgap

I. INTRODUCTION

Due to transparency and strong innature Glasses had attracted more attention than other materials. Glasses have wider applications than crystals since they can be made in any shape, less manufacturing cost and easy modification of properties. Alkali Borosilicate glasses had various applications in optoelectronics. Energy gap (E_g) is an important feature of materials in optoelectronics application.[1-3].

II. EXPERIMENTAL

The compositions of the glass used for the present study is $40SiO_2$ -$30B_2O_3$ –15 Na_2O-15 K_2O.

The glasses used for the present study are prepared by the melting and quenching techniques [4]. The starting materials used for the preparation of the present glasses were analytical grade reagents (99.9 % pure) of SiO_2, B_2O_3, Na_2CO_3 and K_2CO_3. All these chemicals were weighed using electronic balance and were thoroughly mixed in an agate mortar and melted in a porcelain crucible and were melted in a PID temperature controlled furnace at about 950^oC for an half an hour till a bubble free liquid was formed. The resultant melt was poured on a rectangular brass mould (containing smooth polished inner surface) held at room temperature. The samples were subsequently annealed at 450^oC in another furnace.

The obtained glass was then grounded and optically polished to dimensions of 1 cm x 1 cm x 0.2 cm to study the optical properties.

The optical absorption spectra and reflection datawere recorded on a Perkin Elmer lambda 950 UV-VIS-NIR Spectrophotometer in the wavelength range 250 – 1200 nm by DRS technique.

III. RESULTS AND DISCUSSION

Optical band gap is calculated for the present sample by various techniques. The first method is drawing Tauc plots for the analysis of optical absorption spectra.

The following expression was suggested by Tauc [5] and discussed fully by Davis and Mott [6] to calculate optical band gap.

$$\alpha(\nu) = B(h\nu - E_{opt})^n / h\nu$$

where B is the constant and E_{opt} is the energy of the optical band gap and $h\nu$ is the incident photon radiation. For indirect transitions $n = \frac{1}{2}$ and for direct transitions n=2. From the plots of $(\alpha h\nu)^{1/2}$ and $(\alpha h\nu)^2$ as a function of photon energy $h\nu$, E_{opt} values can be obtained by the extrapolation of the linear region of the plots to the $h\nu$ axis for indirect and direct transitions. For lower values of the absorption coefficient the above relation gradually changes into an exponential dependence as given by Urbach law [7].

$$\alpha(\nu) = \alpha(\nu_0)\exp(h\nu/\Delta E)$$

where $\alpha_{0\ iis\ a}$ constant and ΔE is the Urbach energy which indicates the width of band tail of the localized states in the bandgap. Plots are drawn with $\ln(\alpha)$ against $h\nu$ for the glasses to calculate the Urbach energy. The values of Urbach energy are calculated by determining the slopes of the linear regions of the curves and taking their reciprocals.

With the help of kubelka –Munk transformed reflectance spectra also band gap of present mixed alkali borosilicate glass was calculated.
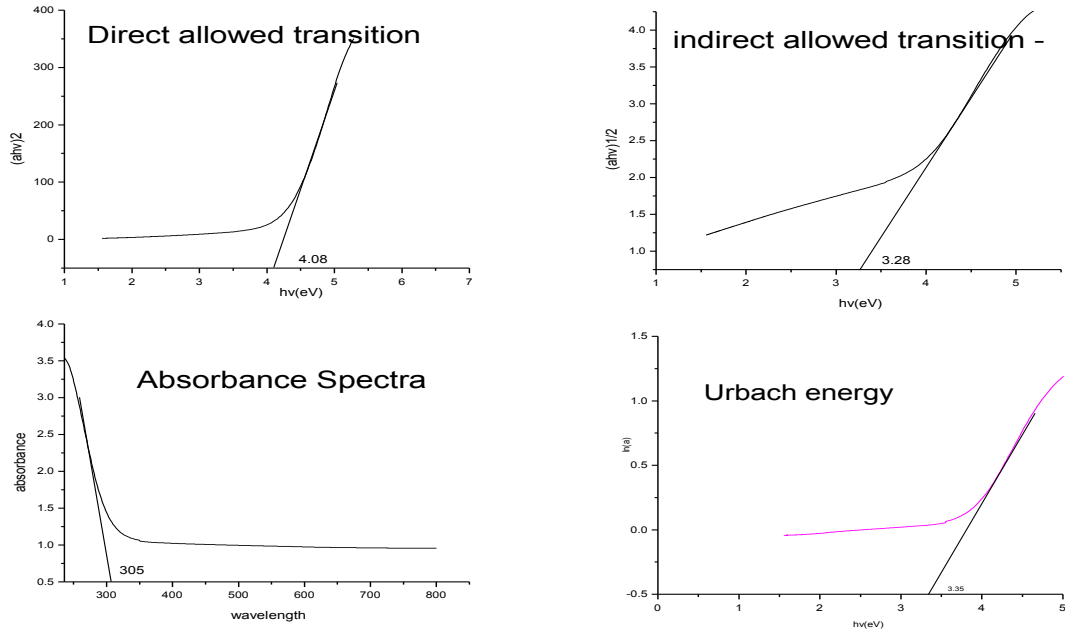
Figure 1 . Band gap- TaucAbsorbance Plots

Band gap is also calculated from diffuse reflectance spectrum using Kubelka- Munk function [8].   Here the relational expression becomes

$$F(R_\infty) = B \ (h\nu - E_g)^n \ /h\nu$$

For indirect transitions $n = \frac{1}{2}$ and for direct transitions n=2 same as discussed for absorption Tauc plots.
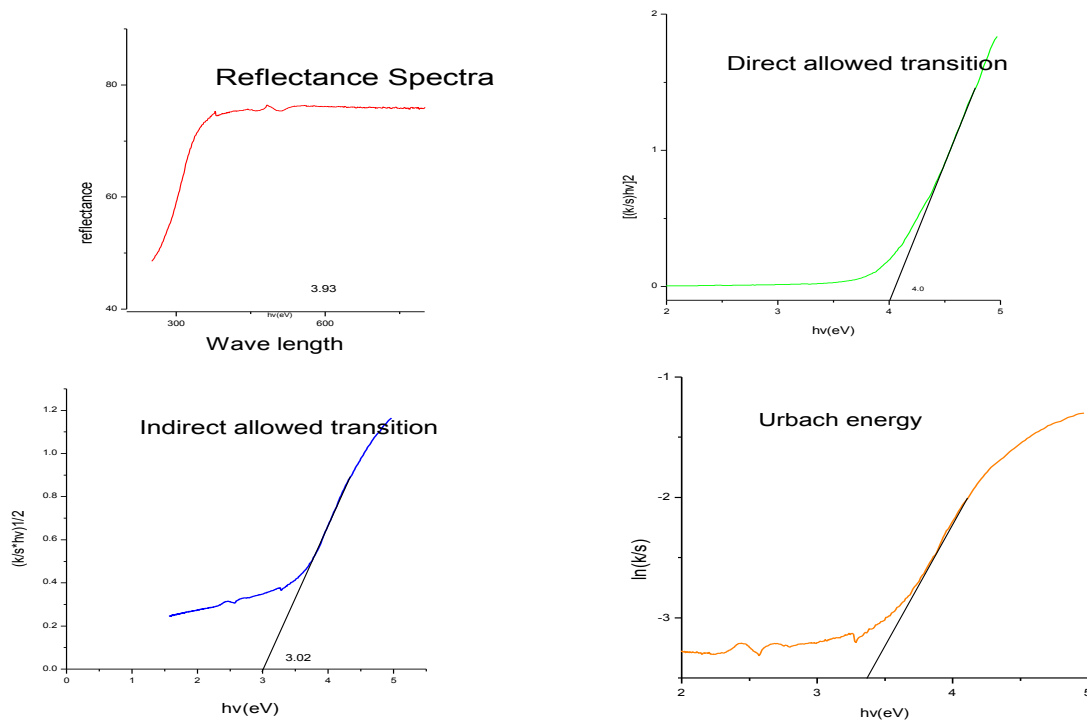

Fig 2. Band gap- Kubelka –munk transformed reflectance Spectra

Another very common method to calculate band gap is from absorption spectra is to get the first derivative of absorbance with respect to photon energy and finding the maxima in the derivative spectra at the lower energy sides [9]. The energy gap is associated to the maximum in the spectrum.
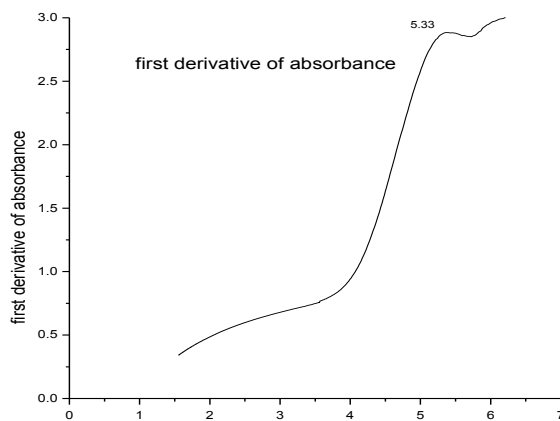

Figure 3: First derivative absorption curve

Band gap values calculated using various methods are shown in Table 1.

Table 1: Comparison of Band Gaps

Glass composition	Indirect band gap (eV)		Direct band gap(eV)		Band gap 1st order derivative Plot (eV)	Urbach energy (eV)	
	Kubelka–munk plot	Tauc plot	Kubelka –munk plot	Tauc plot		Tauc plot	Kubelka –munk plot
SiO_2-B_2O_3-Na_2O-K_2O	3.02	3.28	3.93	4.08	5.15	0.26	0.34

VI CONCLUSION

UV-Vis Absorption technique is most suitable technique to find the band gaps for transparent materials like glass. DRS technique is also convenient technique when polished glass samples are not available and only powder samples are present. The band gap values are same for the present SiO_2 – B_2O_3 –Na_2O - K_2O glass sampleusing both the above methods. First derivative absorption curve does not give accurate value for band gap value.

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