STUDIES ON THE INFLUENCE OF FE_2O_3 ON REFRACTIVE INDEX AND OPTICAL ABSORPTION PROPERTIES OF LITHIUM BOROSILICATE GLASSES.

Thomas Philip
Hislop College, Nagpur – 400 001, India

Abstract

Glass is a viable material for making devices. It is isotropic, less denser stable materials. It is non-crystalline amorphous solid. The lower coefficient of thermal expansion makes them subjected to less stress due to thermal expansion which reduces damage to the material. Glass material is used in different applications like reinforced plastics, fiber optic waveguides in communication networks etc. In the present work, transition metal oxide is added to study the optical properties of the glass system. Compounds of transition metals and rare earths are the most commonly used as dyes. The colour of the glass samples depends on electron structure of the transition metal ions as well as on the chemical composition and structure of the base glass which determines the local site of these elements. The glass samples studied here is represented by general formula $30LiO_2$: $(70\text{-}X)(6/7B_2O_3{:}1/7SiO_2)$: X Fe_2O_3, were synthesized by conventional quenching technique. The study of optical properties of refractive index for X=0.0, 0.5, 1.0, 2.5, the optical absorption for X = 0.0, 0.5, 2.5 and the band gap for X = 0.0, 0.1 of the glasses have been carried out. The refractive index studies have been done by using Abbe refractometer and the AvaSpec Fiber optic spectrometer for optical absorption studies. The refractive indices and absorption band observed for the glass systems have been recorded. The optical band gaps for the above glass samples were calculated from the absorption edge using Tauc plot. It has been observed that the addition of transition metal oxide reduces the optical band gap. The result shows that there are absorptions in the specific wavelengths of the UV- Visible range. These glass systems can be studied further for developing suitable devices.

Keywords: Refreactive Index, Optical absorption, Optical band gap, Tauc plot

1 Introduction

Lithium conducting glasses are prospective electrolyte materials for solid state batteries and have been studied widely in last few decades [1]. When the transition metal oxides are added in glass system, it gives different colouring mechanism. The base glass structure and the electron structure of the transition metal ions determine the colour of the glass. Transition Metal ions are also used as a probe of the glass structure [2,3]. The UV/VIS spectroscopy is a simple experimental technique for the study of colored glasses. The valences and coordination of transition metals in glass can be understood on the analysis of electron spectra. The absorbance of light has been studied by comparing the intensities of light passing through the sample before (I_0) and after (I). The ratio of I/I_0 is called the transmittance. When the transition metal oxides are added into the base material, the molecular structure is changed. The molecular formulation of the transition metal is significant for the optical absorbance study. In general three types of energies are considered. i.e. Electronic, vibrational and rotational energies of the molecule. For electronic transition, high energy photon is required to excite a molecule from lower to higher level. Comparatively lower energies are required for excitation in vibrational and rotational levels. Vibrational and rotational levels are more closely spaced. The plot of absorbance against the wavelength of the incident radiation is expected that it should show sharp lines. Each line should occur when an incident photon of energy exactly

matches with the energy corresponding to the line in the spectrum. Instead of sharp lines, it is found, in practice, few humps. It shows that the molecule is absorbing radiation over a band of wavelengths. The reason for this band can be attributed, rather than line absorption, to simultaneous change between many vibrational levels along with electronic level transitions. The vibrational level can also be associated with smaller rotational changes. The rotational transition energies fill the gaps in the vibrational energy levels. Refractive index is an important optical parameter. It is related to the wavelength of the light used. Optical properties of a few transition metal oxide doped glass systems have been studied earlier[4-5]. However, systematic investigations in this regard are still lacking. Hence in the present work, the influence of Fe_2O_3 addition on the optical properties of lithium borosilicate glass have been studied.

Experimental methods:

The Glasses studied in the present work can be represented by the general formula $30Li_2O$: XFe_2O_3: $(70 - X)(1/7\ SiO_2{:}6/7\ B_2O_3)$ where X = 0.0, 0.1, 0.5, 1.0, 2.5. The finely mixed powders of Li_2CO_3, Fe_2O_3, B_2O_3, SiO_2 of high purity (>99.5%) were melted in platinum crucible at 1100^0C for one and a half hour. The melts were stirred from time to time to attain homogeneity and quenched in an aluminum mould at room temperature in air. The glasses so prepared were annealed for two hours.

The optical absorption studies were done with the help of Avaspec spectrometer in the wavelength range from 200nm to 1000nm. Refractive index studies were done by abbe Refractometer. The densities of these samples were measured by Archimedes' Principle with toluene as immersion liquid. The optical band gaps calculated from the UV absorption edge using Tauc plot.

Results and Analysis

1.Density and Refractive index studies

Density is an index to rigidity of the structure of glass. In the network of the primary glass forming oxides, there are large numbers of interstices. The modifier ions can get stuffed into these interstices. This can increase the mass of the substance without an increase in the bulk volume and it results in an increase in density. The density is direct reflection of glass structure. It is the measure of the rigidity of glass structure which depends on the atomic arrangement., nature, and content of various structural groups and phases present in the glass. The density as a function of composition gives useful information.

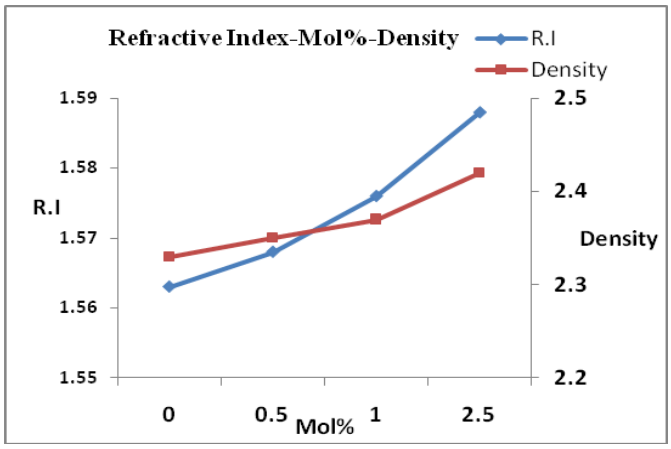


Fig.1. Refractive Index and density results of Fe_2O_3 content at levels X=0.0, 0.5, 1.0, 2.5.

Refractive index is an important optical parameter in determining the applicability of the material in optical devices in telecommunication[6]. The refractive index is closely related to the electronic polarizability and the local field inside the material. Figure 1 illustrates the variation of refractive index and density. Both values are increasing with Fe_2O_3 content. Increase in density shows strengthening of glass network by the tetrahedral formations in the structure. It supports the reduction in the non-bridging oxygen causing less mobility of ions in the network. Refractive index is a wavelength dependent parameter and the values are measured by Abbe Refractometer at 589nm wavelength. When light passes from a rarer medium to denser medium its velocity decreases and then the refractive index of the medium increases. Similar results have been reported for lithium borate glasses. So the

experimentlal values of refractive index and density are mutually agreeing and the measurements have been done for X = 0.0, 0.5, 1.0, 2.5.

2.Optical absorptions studies

The absorption of light in a glass sample depends on the different energy levels associated with a molecule of the substance and it is the sum of the energy of its electrons, vibrational energy between its constitutional atoms and the rotational energy of the molecule

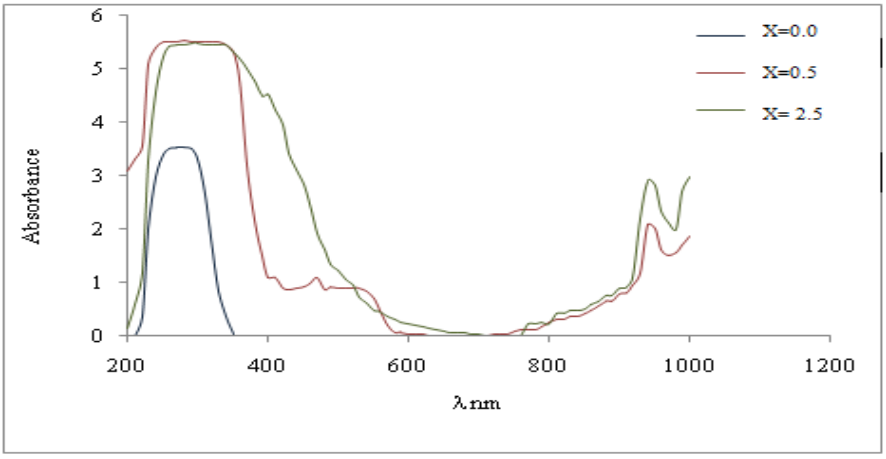
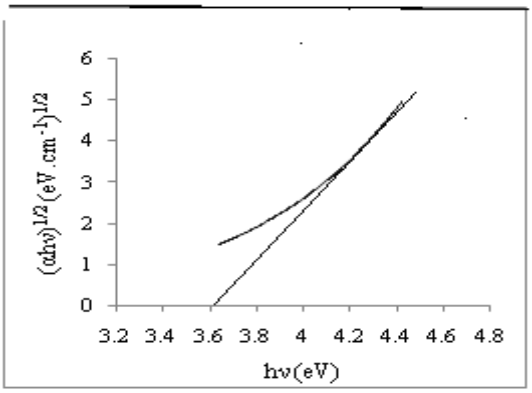


Fig. 2 Variation absorption and wavelemgth with Fe_2O_3 added at levels at X=0.0, 0.5, 2.5

Figure 2 depicts the variation of Absorption and wavelength of the samples of Fe_2O_3 added at levels X=0.0, 0.5, 2.5. When Fe_2O_3 content is increased there is a complete absorption of UV lines and also two weak absorption at 520nm, 410nm peaks in visible region are seen. The broadening of UV absorption band is also observed[7]. Similar results have been reported in the sodium borosilicate glasses containing Fe_2O_3 It is due to the presence of Fe^{3+} States of the Fe-ions. Fe^{3+} ions are expected to occupy tetrahedral positions in the glass matrix[8]. Absorption at 920nm is due to Fe^{2+} ions. Intensity of the lines are increased when Fe_2O_3 content is increased.

3.Optical band gap studies

The Figure 3 and 4 show the tauc plots for the glass samples X =0.0, X=0.1. The optical band gaps for the above glass samples were calculated from the absorption edge using well known Tauc law equation. It shows the relation between 'αhν' and 'hν'. 'B' and 'm' are the parameters in the equation, where hν is the incident photon energy, B is the constant that depends on the electronic transition probability and the 'm' is a parameter which depends on the type of electronic transition responsible for the absorption. The exponent m = ½ for allowed direct transition, where m = 2 for allowed indirect transition [9-11]. The graphs are drawn between 'αhν' and 'hν',which are shown in the plots. By extrapolating the linear portion of the curves to zero absorption, the optical band gaps were determined. It can be observed that the addition of transition metal oxide reduces the optical band gap. To understand the reasons for qualitative and quantitative changes in band gap due to TMO addition, further detailed investigations are needed.



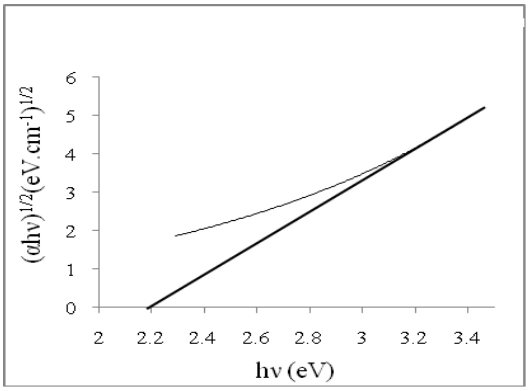


Fig.3: Tauc plots for glass samples X = 0.0

Fig.4: Tauc plots for glass samples X = 0.1

Conclusions

The Fe_2O_3 added lithium borosilicate glass samples were prepared and confirmed by X-ray diffraction. Refractive index and density plots show that both values are increasing. It supports tetrahedral formation in the glass network. In the optical absorption studies, two weak absorption at 410nm and 520nm in the visible region are seen. It is because of the transition in the Fe^{3+} energy levels. The tauc plots results indicate the addition of transition metal oxide reduces the optical band gap in the glass samples. These glasses can be studied in more details to explore them for practical applications.

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