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Physical, structural and optical characterization of silicate modified bismuth-borate-tellurite glasses

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ABSTRACT

The quaternary glass system $xSiO_2$-(80-x) Bi_2O_3–$15B_2O_3$–$5TeO_2$ has been prepared by melt-quench technique. The amorphous nature of glass samples has been ascertained by X-ray diffraction patterns. The variations in density, molar volume and crystalline volume with glass compositions have been discussed. A non-linear change has been observed in glass transition temperature and optical band gap energy. Raman and FTIR spectral studies suggest that glass network is mainly built up of BO_3, BO_4, SiO_4, and TeO_3 structural units, whereas BiO_3 exists as both network modifying [BiO_6] octahedral as well as network forming [BiO_3] pyramidal structural units. The values of optical band gap energy have been estimated from fitting of both Mott and Davis's model and Hydrogenic excitonic model (HEM) with experimental data of absorption spectra. The HEM model shows good agreement with experimentally observed absorption spectra, which indicates the exciton formation in studied glass system. The non-linear compositional change in optical band gap energy is related with the structural changes occurring in present glass samples. The Urbach energy has also been estimated. The range of metallization criterion suggests that prepared glasses may be considered as new nonlinear optical materials.

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1. Introduction

Recently, structural and optical properties of Bi_2O_3 based oxide glasses have been studied vastly [1–9] because of its role as both network former and modifier. These glasses have interesting application as transmitting windows in IR region, photocatalytic degradation materials, thermal and mechanical sensors and layers for optical and electronic devices [5,9–12]. B_2O_3 is one of the basic glass formers and mainly exists in the form of trigonal BO_3 and tetrahedral BO_4 units. It forms glass at lower temperature with good transparency, high chemical durability and thermal stability [13,14]. Bismuth borosilicate glasses are important in the present because of their useful luminescent and non-linear optical properties [12,15,16]. Tellurite glasses are important due to their promising optical properties such as high linear and non-linear refractive indices, low melting point and good transmission in IR regions [5,17,18].

Silicate glasses are chemically durable, thermally stable and optically transparent at excitation and lasing wavelength [19]. In addition, high viscosity of these glasses allows the glass to be formed, cooled and annealed without crystallization. They are useful in optics as lenses or beam splitters, in optical telecommunications, micro- and optoelectronics and in near IR-windows [20,21]. A review of literature shows that there are many reports on B_2O_3: Bi_2O_3: SiO_2 [22], TeO_2: Bi_2O_3: SiO_2 [18], Bi_2O_3: SiO_2: Fe_2O_3 [4], TeO_2: Bi_2O_3: B_2O_3: ZnO [5] and TeO_2: Bi_2O_3: B_2O_3: PbO [17] glass systems. But there is hardly one report on Bi_2O_3: B_2O_3: TeO_2: SiO_2 [8] glass system, where we studied effect of B_2O_3 on Bi_2O_3: TeO_2: SiO_2 glass system and noticeable change in physical, structural and optical properties has been observed on addition of borate to bismuth tellurite silicate glass system.

To optimize Bi_2O_3: B_2O_3: TeO_2: SiO_2 glass system for use as non-linear optical material and in order to explore its technological applications, the effect of SiO_2 on physical, structural and optical properties of bismuth-borate-tellurite glasses have been studied and reported in present manuscript.

2. Experimental details

2.1. Glass preparation

Glass samples of compositions $xSiO_2$-(80-x) Bi_2O_3–$15B_2O_3$–$5TeO_2$, with x = 0, 5, 10, 15, 20, 25 and 30 were prepared

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by conventional rapid melt-quenching technique using analar grade chemicals H_3BO_3, TeO_2, Bi_2O_3 and SiO_2. The raw materials in appropriate molecular ratios were thoroughly mixed in an agate pestle mortar to form batches of 20 g. The batch mixture was then melted in a porcelain crucible in an electrically heated muffle furnace under ordinary atmospheric conditions at a temperature of about 1100 °C which was kept for 1 h and the melt was occasionally swirled to ensure proper mixing, homogeneity and to avoid the presence of bubbles. Finally, the glasses were formed by pouring the melt at room temperature on to a stainless steel block and it was quickly quenched by pressing with another stainless steel block. The as prepared samples were annealed at 350 °C (below its glass transition temperature) for four hours to minimize the internal mechanical stress (which may have developed during the quenching process) and subsequently cooled to room temperature in furnace.

2.2. Glass characterization

The amorphous nature of glass samples was ascertained by X-ray diffraction patterns using Rigaku Table-Top X-ray Diffractometer with Cu–Kα radiation (λ = 1.54 Å) at 30 KV and 15 mA in 2θ range 20°–80° with a scanning rate of 4° per minute. The density (ρ) measurements were made by the Archimedes' method using SI-234 Denver Instrument with xylene as buoyant liquid. The glass transition temperature (T_g) of samples was measured by differential scanning calorimetry (DSC) technique using TA (thermal analysis and analyzers) instrument, model No.Q600 SDT, with a heating rate of 20℃/min in temperature range 200 °C–800 °C in nitrogen atmosphere. The IR spectra of powdered glass samples were recorded at room temperature using KBr pellet technique on a Shimadzu IRaffinity-I 8000 FTIR spectrophotometer in wavenumber range 400 cm^{-1} -1500 cm^{-1} with spectral resolution of 2 cm^{-1}. The powdered glass samples were thoroughly mixed with dry KBr in a ratio 1:20 by weight and then pellets were formed under a pressure of 10^9 Pa to produce clear homogenous discs. The room temperature Raman measurements of the polished samples were performed on Renishaw Invia Reflex Micro Raman Spectrometer with Ar ion laser (514 nm) under back scattering configuration in the range 100 cm^{-1} -1700 cm^{-1} with spectral resolution of 1 cm^{-1}. Laser power at the sample was ~100 mW and typical acquisition time was 30 s. FTIR and Raman spectra were found to be consisting of a group of broad bands that are composed of a number of overlapping peaks. To resolve these peaks and to find out the expected exact position of peaks, deconvolution of FTIR and Raman spectra was performed using "multiple peaks fit" module of Origin Pro 8.6 software by using Gaussian function. The quality of Gaussian fitting is evaluated by best fit parameter R^2 and in present case R^2 is greater than 0.9999. The statistical validation has also been tested by applying F-test following the procedure reported earlier [3,6,23]. The optical absorption spectra of prepared glass samples were recorded at room temperature using 3100 MC Shimadzu UV–Vis. spectrophotometer in the wavelength range 200 nm–800 nm with spectral resolution of 1 nm and spectral slit width of 2 nm.

3. Results and discussion

3.1. XRD analysis

X-ray diffraction (XRD) patterns of prepared glass samples presented in Fig. 1 exhibit broad diffuse scattering around low angle region, instead of sharp crystalline peaks, which ensure the amorphous nature as well as absence of long range atomic arrangement in studied glass samples.

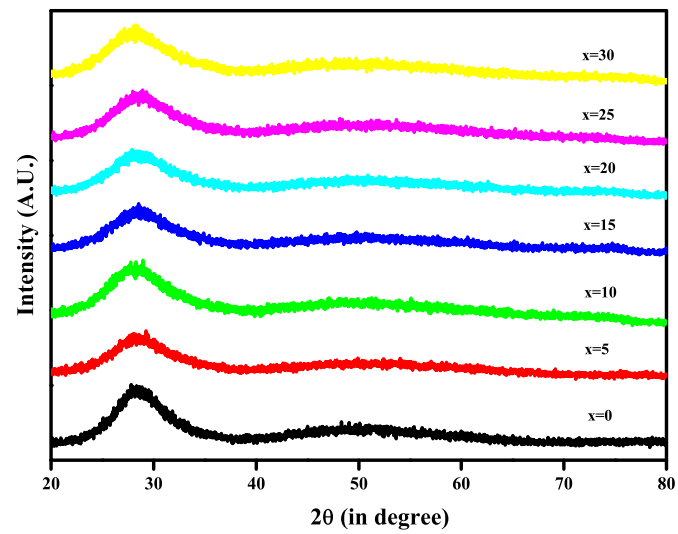

Fig. 1. X-ray diffraction patterns of different $xSiO_2$-(80-x) Bi_2O_3–$15B_2O_3$–$5TeO_2$ glass compositions.

4. Density, molar volume and equivalent crystalline volume

The density for all glass samples was measured using Archimedes' principle and corresponding molar volume (V_m) of samples was calculated using the relation [1]:

$$V_m = \sum x_i M_i / \rho \quad (1)$$

where x_i, M_i are respectively the molar fraction and molecular weight of the ith component and ρ is the density of the sample. Their values are listed in Table 1. Perusal of data presented in Table 1 show that density and molar volume of the samples decrease from 5.995 g/cm^3 to 5.697 g/cm^3 and 65.06 cm^3/mol to 47.09 cm^3/mol, respectively with increase in SiO_2 content at expense of Bi_2O_3 content. The decrease in density is an expected result as heavier Bi_2O_3 (atomic mass 465.95) is being replaced by lighter SiO_2 (atomic mass 60.09). The decrease in molar volume with increase in SiO_2 content is mainly attributed to smaller radii and bond lengths of SiO_2 than that of Bi_2O_3 and thus results in a shrinking of free volume [24]. Further, according to Pan et al. [25], SiO_2 tetrahedral can be incorporated in the network of more flexible structure of bismuth-oxygen polyhedral, $[BiO_n]$ due to more ionic nature of Bi–O bond and hence the decrease in molar volume in presently studied glasses.

The corresponding molar volume for their crystalline phases or equivalent crystalline volume (V_c) of the glass samples is given by the formula [1]:

$$V_c = \sum x_i V_i \quad (2)$$

where V_i is molar volume of the ith component in crystalline phase. The calculated values of V_c are included in Table 1. The data of molar volume and equivalent crystalline volume are compared in Fig. 2, which in turn shows that values of V_m of glasses for different compositions are greater than the corresponding values of the V_c, indicating that structure of non-crystalline counter part of these mixed crystalline phases are expanded with some excess structural volume.

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