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Optical and structural evaluation of bismuth alumina-borate glasses doped with different amounts of (Y_2O_3)

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ABSTRACT

Network of new quaternary borate glasses Bi_2O_3–Y_2O_3–Al_2O_3–B_2O_3 was studied by FTIR and UV spectroscopies. According to the FTIR results, the addition of Y_2O_3 increases the amount of bridging oxygens and changes the coordination number of the glasses by creating [BO_4] structural units. FTIR investigations explained the increase of the computed elastic moduli according to Makishima–Mackenzie model. The optical parameters such as the UV transmission, the polarizability, and the basicity are found to be sensitive to the concentration of Y_2O_3. The results of the elastic moduli and the optical parameters were interpreted in terms of the vibrations of structural groups and the strength of the bonds.

1. Introduction

Recently, rare-earth doped glasses draw the attention due to their considerable scientific and technological interests that arise from the transitions of 4f–4f and/or 4f–5d in the electronic configurations of the luminescent dopants [1]. These glasses are considered as promising candidates for optical amplifier media, tunable laser devices and can be used as luminescence materials in the optical communications channels [2].

The physical properties of the glass depend on its composition and can be correlated with the interatomic forces and the potential of the local structure. Thus, adding a modifier led to change the properties and the energy band gap of the glass network [3–4]. In general, glasses with more bridging oxygens (BOs) have a strengthened glass structure, high elastic moduli, and high optical band gap [4]. The elastic moduli depend on the average bond dissociation energies of the incorporated oxides in the glass network. Moreover, investigation of the optical properties of the glass network and its structure–relationship is one of the most fruitful procedures to understand the glass band structure and its energy gap [1].

On the other hand, intermediate oxides such as Al2O3 or Y2O3 can act either as glass modifier or glass former, depending upon their concentration in the glass network composition [5]. Y_2O_3 increases the efficiency of hole burning [6], enhances the physical stability, the intensity of broadband NIR emissions [7] and the mechanical strength of the host glass material [8]. Kaur et al. [5] reported that the optical band gap decreases whereas optical basicity increases with increase in Y2O3 content of SiO2-BaO-xB2O3-(10-x) Y2O3 system. Al_2O_3 decreases the devitrification of the glass network, improves the glass forming tendency and increases the coefficient of thermal expansion. Furthermore, Bi_2O_3 has a great interest not only due to its long infrared cut-off but also due to its highly polarizability, density and refractive index [8–10].

In the present work, $(Bi_2O_3)_{0.6}$–$(Y_2O_3)_x$–$(Al_2O_3)_{0.1-x}$–$(B_2O_3)_{0.3}$ ($0 \le x \le 0.1$ mol fraction) glass system has been synthesized and characterized using FTIR, and UV–vis spectroscopy techniques. The physical parameters, optical band gap, and computed elastic moduli according to Makishima–Mackenzie model have been obtained to explore the influence of Y_2O_3 on structural and optical properties of borate based glasses.

2. Experimental procedures

Different glass compositions with the chemical formula $(Bi_2O_3)_{0.6}$–$(Y_2O_3)_x$–$(Al_2O_3)_{0.1-x}$–$(B_2O_3)_{0.3}$ ($x = 0, 0.02, 0.04, 0.06, 0.08$ and 0.1 mol fraction) were synthesized. Analar grade Bi_2O_3, Al_2O_3, Y_2O_3, and H_3BO_3 were mixed to give the mentioned nominal compositions [Table 1]. The mixed batches were melted in an electric furnace at 1100 °C for 4 h using a covered Pt–Rd 10% crucible then, casting into a steel mold to produce bulk glasses and annealed at a temperature of ~350 °C. The bulk glasses with thickness 0.1 cm were polished for

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Table 1
Deconvolution parameters of the infrared spectra of glasses of the glasses $(Bi_2O_3)_{0.6}$–$(Y_2O_3)_x$–$(Al_2O_3)_{0.1-x}$–$(B_2O_3)_{0.3}$,$(0 \le x \le 0.1$ mol). *C* is the component band center (cm^{-1}) and *A* is the relative area (%) of the component band.

0 Y_2O_3		0.02 Y_2O_3		0.04 Y_2O_3		0.06 Y_2O_3		0.08 Y_2O_3		0.1 Y_2O_3	
A	*C*	*A*	*C*	*A*	*C*	*A*	*C*	*A*	*C*	*A*	*C*
4.7	406	3.2	452	2.3	447	5.2	455	2.9	454	3.1	453
28.4	515	14.9	528	15.0	526	17.5	557	14.9	534	11.4	530
4.4	710	4.3	709	3.6	707	4.9	709	3.9	705	2.3	705
15.7	852	25.7	884	25.4	880	17.6	844	25.5	871	27.4	873
11.2	943	9.9	1000	11.4	993	14.4	944	14.3	985	16.7	1003
7.9	1030	5.4	1074	6.3	1069	10.7	1043	6.3	1064	11.7	1082
9.6	1171	6.9	1186	12.3	1192	9.5	1192	11.3	1192	7.7	1204
13.5	1268	18.7	1269	19.2	1299	14.8	1295	16.1	1295	13.8	1296
4.6	1358	11.0	1367	4.5	1383	5.4	1355	4.8	1375	5.9	1378

density and UV–VIS measurements and small pieces of the same samples were crushed and pulverized for FTIR measurements.

A Philips X-ray diffractometer (XRD) PW/1710 with Ni-filtered, Cu-Kα radiation (λ = 1.542 Å) powered at 40 kV and 30 mA were used to check the amorphous state of glasses. Fourier Transform Infrared (FTIR) spectroscopy was carried out at room temperature in the region 400–2000 cm^{-1} using infrared spectrophotometer type JASCO, FT/IR – 430 (Japan). The spectral resolution of FTIR spectroscopy was ±4 cm^{-1}. A random error in the center of FTIR bands was found as ±2 cm^{-1}. 10 mg of each sample was mixed with 40 mg of KBr in an agate mortar. The IR spectra are corrected for the noises of dark current then, normalized to eliminate the concentration effect of the powder sample in the KBr disc.

Glass density (ρ) was measured using Archimedes technique using toluene as an inundation fluid and the experiment has been carried out five times for each glass sample. A random error in the measured density was found as ±22 kg/m^{-3}. Based on ρ values the molar volume ($V_m = M/\rho$ where *M* is the molar weight of the glass) has been estimated.

The spectra of both UV transmittance (*T*), and reflectance (*R*) of the highly polished glasses are measured at room temperature in the 200–2000 nm spectral range using a computer controlled double beam UV–VIS spectrophotometer (SHIMADZU UV-2100).

3. Results and discussions

The prepared glass samples are transparent, bubble-free and were reddish brown. XRD patterns (not shown here) revealed an only broad humps characteristic of the amorphous nature without any sharp lines or peaks.

3.1. FTIR analysis

Fig. 1 shows the effect of Y_2O_3 on the FTIR spectra of the prepared glasses. The spectra revealed three major broad absorption bands. The first one at ~500 cm^{-1}, the second at 890 cm^{-1} with a shoulder at 985 cm^{-1} and the third band at 1200 cm^{-1} with a shoulder at 1304 cm^{-1} along with a minor absorption band around 705 cm^{-1} for all glasses. The broadness of the bands may be due to the randomness of the glass structure and to the overlapping of the vibrations of specific structural units which affect the density and the optical properties of the glasses under study. A deconvolution process using Origin 8 program was performed to identify the vibrational band of each structural unit. The parameters of the deconvolution process such as the center *C* and the relative area *A* of each specific band were listed in Table 1. Figs. 2–3 depict the bands of deconvolution of the FTIR spectra of the samples having 0 and 0.1 mol of Y_2O_3, respectively which is perfectly convenient with the data from the literature [4].

Accordingly, the bands at 1383–1333 cm^{-1} are relevant to asymmetric stretching vibrations of B—O bonds in $[BO_3]$ triangle, the

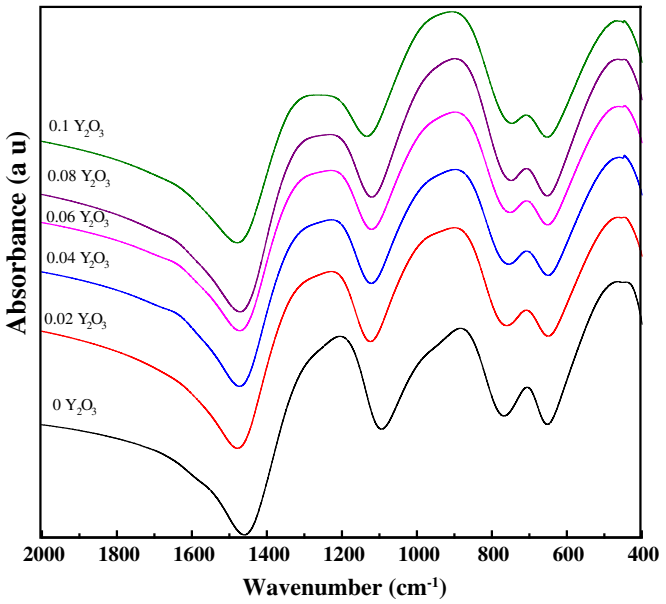

Fig. 1. Infrared spectra of the investigated $(Bi_2O_3)_{0.6}$–$(Y_2O_3)_x$–$(Al_2O_3)_{0.1-x}$–$(B_2O_3)_{0.3}$ glasses. Numbers at the plots represent Y_2O_3 content in mol fraction.

bands at 1299–1219 cm^{-1} are related to B—O and B—O^- stretching vibrations of BO_3 and BO_2O^- units, while the bands at 1204–1157 cm^{-1} are ascribed to stretching vibration of B—O in $[BO_3]$ units from pyro- and orthoborate groups [2,11]. The deconvoluted bands at 1082–1062 cm^{-1} are ascribed to vibrations of $[BO_4]$ structural units from tri-, tetra- and pentaborate groups [12], the bands at 1003–944 cm^{-1} are attributed to the stretching vibrations of B—O bonds in the $[BO_4]$ tetrahedra [13,14] while the bands at 884–844 cm^{-1} are ascribed to symmetrical stretching vibrations of Bi—O bonds of $[BiO_3]$ units [15,16]. The latter bands may be overlapped with the vibrations of $[AlO_4]$ groups [11,17]. The minor absorption bands around 705 cm^{-1} are related to the bending vibrations of B—O—B bonds in $[BO_3]$ groups [18] and overlapped with the stretching vibrations of the Y—O bonds with Y^{3+} ions in four-fold coordination [19,20]. Bands at 557–526 cm^{-1} are ascribed to the presence of structural units $[BO_3]$ and $[BO_4]$ [21] and overlapped with the vibrations of both $[AlO_6]$ octahedral [17] and Bi—O bond in $[BiO_6]$ units [15]. The bands at 455–447 cm^{-1} are attributed to Bi—O valence vibrations of very deformed $[BiO_6]$ units [20].

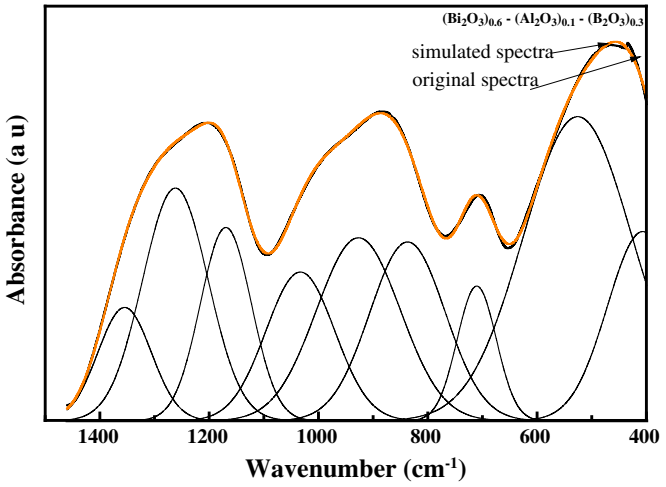

Fig. 2. Curve-fitting of IR spectra of the glass $(Bi_2O_3)_{0.6}$–$(Al_2O_3)_{0.1}$–$(B_2O_3)_{0.3}$.