




A Study of Thermal, and Optical Properties of 22SiO_2 - $23\text{Bi}_2\text{O}_3$ - $37\text{B}_2\text{O}_3$ - 13TiO_2 -(5-x) LiF- x BaO Glasses

Atif Mossad Ali^{1,2} · Z. A. Alrowaili³ · Ateyah M. Al-Baradi⁴ · M. S. Al-Buriah⁵ · E. A. Abdel Wahab⁶ · Kh. S. Shaaban⁷ 

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Abstract

Using melt-quenching techniques, the glass system 22SiO_2 - $23\text{Bi}_2\text{O}_3$ - $37\text{B}_2\text{O}_3$ - 13TiO_2 - (5 - x) LiF- x BaO was prepared. The amorphous status of fabricated samples were established using X-ray diffraction patterns. Differential thermal analysis (glass transition temperature, crystallization temperature, and thermal stability) as well as optical properties (molar refractivity, bandgap, molar polarizability, reflection loss, metallization, electronegativity, and electron polarizability) of these glasses have been investigated. These structural changes influence the thermal properties, as we discovered. Indeed, as BaO levels rise, all the thermal parameters rise as well. With increasing BaO content, density, and refractive index rise. Bandgap energies for direct and indirect transitions reduced as the BaO content increased while Urbach energy increases. This interpretation attributable to the increment in the bond length of Ba-O. This study suggests that the fabricated glasses' optical and thermal characteristics have improved, making them suitable for a variety of applications.

Keywords Titania · Glasses · DTA · UV spectroscopy · Polarizability · Basicity

1 Introduction

Due to their unique physical, mechanical, and chemical characteristics, borosilicate glasses are one of the most examined glasses. These glasses are dopant with a wide range of modifying oxides, like transition metal oxides (TMO), and form strong glass networks. Condensed matter physics, glass science, and materials chemistry are all interested in the

characteristics of these glasses. Many physicists and chemists investigated these glasses using theoretical and experimental methods. By taking the different valence states of bismuth ions, bismuth borosilicate network structures have been improved. Therefore, these glasses are appropriate for electro-optic, protection, and electronic applications [1–5].

Glass with (TMO) has been used in a wide range of applications in recent years due to its unique optoelectronic characteristics [6–9]. TiO_2 is a common glass ingredient used to improve the optics and thermal features of the glass. Small amounts of TiO_2 can have a big impact on mechanical, optical, and shielding properties, which is why glass scientists are interested in it [10–17]. Due to its different coordination states Ti^{+4} , Ti^{+5} , and Ti^{+6} , TiO_2 plays a significant role in glass systems. TiO_2 can have a completely different impact on the characteristics because of the change in coordination [10–17].

Fluoro-alkali- TiO_2 - SiO_2 - B_2O_3 glasses present an attractive structure for observing changes in glass behavior. Infrared spectroscopy, shielding, mechanical, and UV-spectroscopy techniques have been used to investigate the structure of these glasses [18–20]. Alkaline- TiO_2 - SiO_2 - B_2O_3 glasses present an attractive structure for observing changes in glass behavior. TeO_2 - LiNbO_3 - BaO - BaF_2 - La_2O_3 glass system is examined by Rammah et al. for its structural, optical, and shielding

✉ Kh. S. Shaaban
khamies1078@yahoo.com

¹ Physics Department, Faculty of Science, King Khalid University, Abha 61413, Saudi Arabia

² Department of Physics, Faculty of Science, Assiut University, 71516 Assiut, Egypt

³ Physics Department, College of Science, Jouf University, P.O. Box: 2014, Sakaka, Saudi Arabia

⁴ Department of Physics, College of Science, Taif University, P.O. Box 11099, 21944 Taif, Saudi Arabia

⁵ Department of Physics, Sakarya University, Sakarya, Turkey

⁶ Physics Department, Faculty of Science, Al Azhar University, P.O. Box 71524, Assiut, Egypt

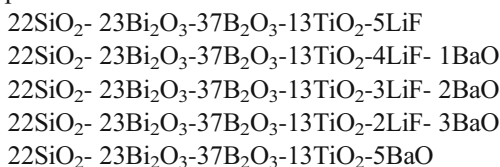
⁷ Chemistry Department, Faculty of Science, Al-Azhar University, P.O. Box 71524, Assiut, Egypt

properties [21]. The structural, optics, and influence of gamma irradiation of the NaF-CaF₂-B₂O₃ glass system are investigated by El Batal et al. [22]. Abd El-Rehim [23] and Shaaban et al. [24] examined the effects of La₂O₃ on the optical, thermal, and radiation characteristics of NaF - BaO - PbO - B₂O₃ glasses.

Using melt-quenching techniques, the glass system 22SiO₂- 23Bi₂O₃-37B₂O₃-13TiO₂-(5 - x) LiF- x BaO was prepared. The effects of increasing BaO content on optical characteristics have been evaluated. *E_{opt}* has been obtained in both linear and non-linear. BaO has increased at the expense of LiF, the extent of thermal in these samples has been investigated.

2 Materials and Methods

The high temperature melting method was used to create the glasses. With mol%, the glasses have the following chemical composition:



For glass preparation, starting materials with purity (99.99 %) were used. Aldrich provides all raw materials used in the production of glasses. H₃BO₃ is converted to B₂O₃ after H₂O evaporation. The reagents were mixed in an electric furnace and then melted for 2 h at 1200 °C in ceramic crucibles. The homogeneous melts were then cast into a graphite mould that had been preheated. At 450 °C, the synthetic samples were annealed.

The structure of the samples was analysed using a Philips X-ray diffractometer (model PW/1710). Using CCl₄ as the buoyant medium, the glass density was determined using the Archimedes principle. A spectrophotometer (JASCO V-670 - Japan) was used to measure the UV transmittance (T) and absorbance (A) spectra of highly polished glasses from 2700 to 200 nm. The molar refractivity *R_m* is expressed as bandgap *E_{opt}*, molar polarizability (α_m), and Reflection loss *R_L*, expressed as: $R_m = V_m \left(1 - \sqrt{E_{opt}/20} \right)$, $\alpha_m = \left(\frac{3}{4\pi N} \right) R_m$, $R_L = \left(\frac{R_m}{V_m} \right)$. Metallization *M*, electronegativity (χ), electron polarizability α° , and optical basicity \wedge expressed as: $M = 1 - \frac{R_m}{V_m}$, $\chi = 0.2688E_{opt}$, $\alpha^\circ = -0.9\chi + 3.5$, and $\wedge = -0.5\chi + 1.7$.

The DTA investigation was conducted using a micro-DTA apparatus (Shimadzu, TA-50, Japan). The measurements are accurate to within 5 °C [25].

3 Results and Discussions

3.1 Physical Investigation

The crystalline, amorphous, and mixed existence of the samples was determined using XRD. XRD of synthesized glasses in the (10–100) 2 θ range is displayed in Fig. 1. Because the XRD of all synthesized glasses was similar, only the XRD for 22SiO₂- 23Bi₂O₃-37B₂O₃-13TiO₂-3LiF-2BaO is shown here. Because of the presence of short-range effects, the hump in the synthesized glass in Fig. 1 indicates that it is non-crystalline. Ensure that the fabricated samples are amorphous consequently.

Molecular weights and densities are commonly used to evaluate glass density [26–30]. BaO was increased in this study at the expense of LiF. BaO and LiF have molecular masses (153.326 & 25.939), and densities (5.72 & 2.64 g/cm³). Therefore, density of these samples was increased, as have been reported. The decrease in *V_m* could be linked to the establishment of (BO), which lessen voids within the structure. ρ & *V_m* of 22SiO₂- 23Bi₂O₃-37B₂O₃-13TiO₂-(5 - x) LiF- x BaO glasses are depicted in Fig. 2.

The values of (*R_m*), (α_m), (*R_L*) and (χ), decline with Ba⁺², owing to the decrease in *V_m*, whereas *M* increases. α° and \wedge have the dissimilar value of (χ), so α° and \wedge reduces as Ba⁺² increases. The obtained data values are shown in Table 1.

3.2 Optical Studies

The reflectance (R) has been estimated based on both the optical absorption (A) and transmittance (T). Absorption (A) and transmittance (T) of a glass system are depicted in Fig. 3. The reflectance (R) of fabricated samples is represented in Fig. 4.

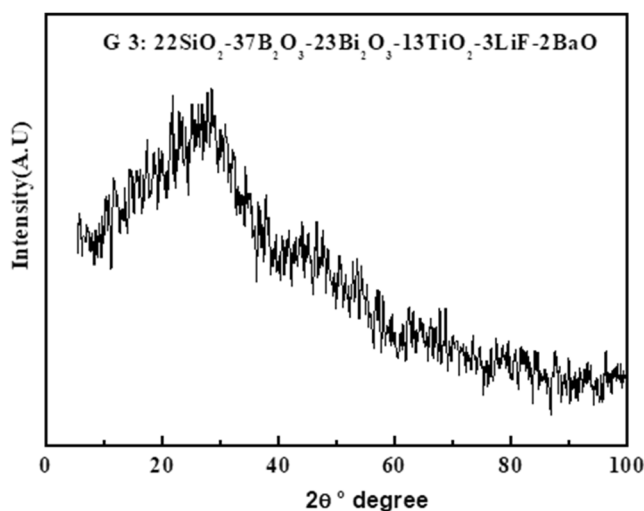


Fig. 1 XRD of 22SiO₂- 23Bi₂O₃-37B₂O₃-13TiO₂-3LiF- 2BaO glasses

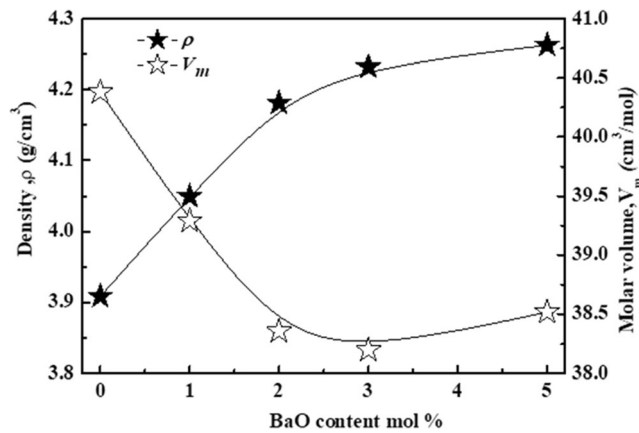


Fig. 2 ρ & V_m of $22\text{SiO}_2\text{-}23\text{Bi}_2\text{O}_3\text{-}37\text{B}_2\text{O}_3\text{-}13\text{TiO}_2\text{-(}5-x\text{) LiF-x BaO$ glasses

These observations were used to evaluate the absorption coefficient (α), linear & nonlinear bandgap (E_{opt}) Urbach energy (E_U), refractive index (n_D). (α), of these glasses were estimated as: $\alpha = (2.303/d) * A$ where d is the sample's thickness. (α), of these glasses was exemplified in Fig. 5. Figure 5 shows an increment as BaO concentration increments, but a decline as light energy increment.

Bandgap energies for direct and indirect transitions, according to Tauc's theory [31–36] are evaluated by: $\alpha h\nu = C (h\nu - E_{opt})^s$. Figs. 6 and 7 present the correlation between $(\alpha h\nu)^{1/2}$, $(\alpha h\nu)^2$, and $(h\nu)$. The intercepts were used to calculate E_{opt}^{dir} , and E_{opt}^{indir} for the examined glasses. The obtained data values are shown in Table 1. E_{opt}^{dir} , and E_{opt}^{indir} both reduced as the BaO content increased. This interpretation may be attributable to the increment in the bond length of Ba-O (1.9397Å) than Li-F (1.57 Å).

E_U of glasses has expected as: $\alpha_0 \exp\left(\frac{h\nu}{E_U}\right) \cdot \ln(\alpha)$ versus $(h\nu)$, is used to calculate the (E_U) in Fig. 8. The varying

Table 1 Physical characteristics of $22\text{SiO}_2\text{-}23\text{Bi}_2\text{O}_3\text{-}37\text{B}_2\text{O}_3\text{-}13\text{TiO}_2\text{-(}5-x\text{) LiF-x BaO$ glasses

Samples	G 1	G 2	G 3	G 4	G 5
N_O	2.5	2.51	2.52	2.53	2.55
R_m (cm ³ /mol)	24.3	23.8	23.5	23.61	24.58
α_m (Å ³)	9.65	9.46	9.34	9.366	9.749
(R_L)	0.6	0.61	0.61	0.618	0.638
(M)	0.4	0.39	0.39	0.382	0.362
(χ)	0.85	0.83	0.802	0.784	0.704
(α°)	2.74	2.75	2.78	2.795	2.87
(ρ)	1.28	1.285	1.3	1.31	1.35
E_{opt}^{indir} (e.V)	3.16	3.09	2.985	2.915	2.62
E_{opt}^{dir} (e.V)	3.52	3.31	3.22	3.19	2.82
E_U (eV)	0.339	0.357	0.367	0.376	0.398

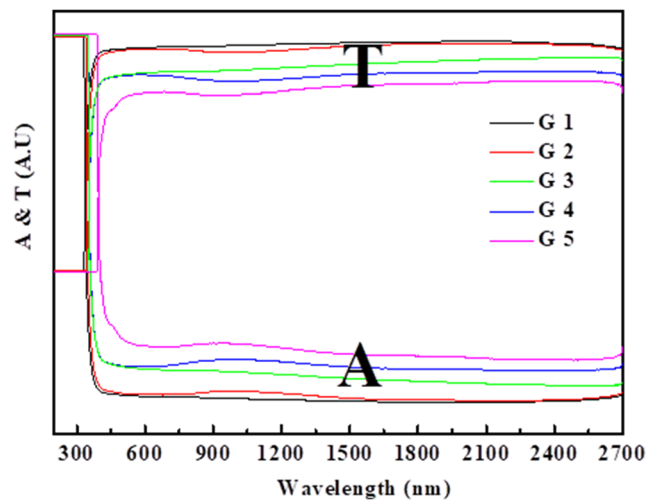


Fig. 3 T & A of $22\text{SiO}_2\text{-}23\text{Bi}_2\text{O}_3\text{-}37\text{B}_2\text{O}_3\text{-}13\text{TiO}_2\text{-(}5-x\text{) LiF-x BaO$ glasses

relationship stated among their E_{opt} belongs to E_U . As BaO increases, the E_U increases while the E_{opt} decreases, as shown in Fig. 8; Table 1.

Manufacturing glasses have a refractive index as: $n_D = \frac{(1-R)^2 + k^2}{(1+R)^2 + k^2}$ where $k = \alpha\lambda/4\pi$, and R reflectance and presented in Fig. 9. With increasing BaO content, n_D increases linearly due to increment of density. It stated that ρ and n_D have a meaningful correlation, i.e., the denser the higher n_D value.

Molar Refractivity $R_m = \langle n^2 - 1 | n^2 + 2 \rangle V_m$, molar polarization

$$\alpha_m (3|4\pi N) R_m, \text{ polarizability } \alpha_0^2 = \frac{\left[\frac{V_m}{2.52} \left(\frac{n^2-1}{n^2+2} \right) - \sum \alpha_{cat} \right]}{N_0^2}$$

, and optical basicity = $1.67 \left(1 - \frac{1}{\alpha_0^2} \right)$ were determined. Figures 10 and 11, and 12 illustrate these concepts. These constructs increase as increment BaO concentration,

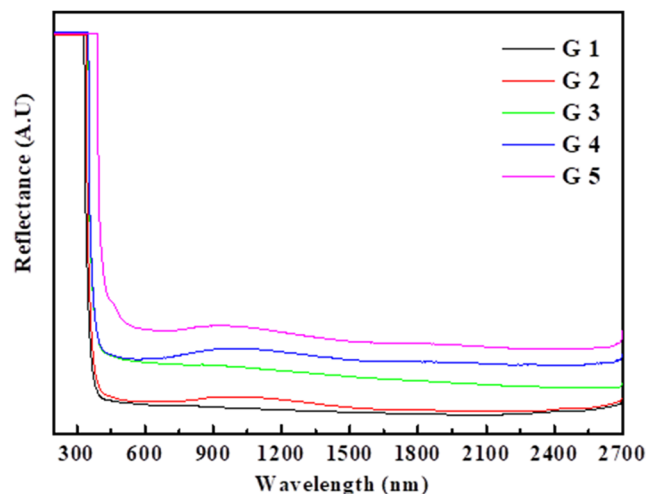


Fig. 4 R of $22\text{SiO}_2\text{-}23\text{Bi}_2\text{O}_3\text{-}37\text{B}_2\text{O}_3\text{-}13\text{TiO}_2\text{-(}5-x\text{) LiF-x BaO$ glasses

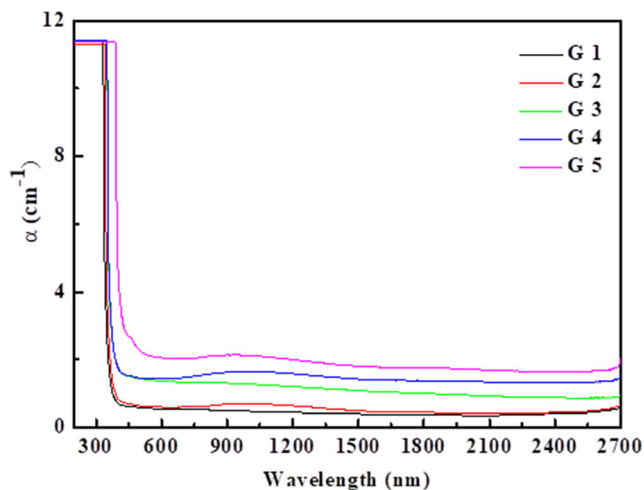


Fig. 5 α , of $22\text{SiO}_2\text{-}23\text{Bi}_2\text{O}_3\text{-}37\text{B}_2\text{O}_3\text{-}13\text{TiO}_2\text{-(}5-x\text{) LiF-x BaO}$ glasses

according to the results of these glasses. The R_m , α_0^{2-} , and of having the same direction of $R_{\text{and}n_D}$. As a result of the increase in BaO, these samples are more polarized. R_m , α_0^{2-} , and values are increased due to higher polarizability of BaO (3.652) than LiF (3.099) [37–40].

E_o and E_d dispersion was determined by [39–42], $n^2 - 1 = \frac{E_o E_d}{E_o^2 - E^2}$. The slope and intercept of Fig. 13 predict E_o and E_d . E_{opt} , (n_o) , ϵ_∞ , (λ_o) , and (S_o) were calculated as: $E_{opt} = \frac{E_d}{2}$, $n_o = \sqrt{1 + \frac{E_d}{E_o}}$, $\epsilon_\infty = n_o^2 \text{ and } n^2 - 1 = \frac{S_o \lambda_o^2}{1 - (\frac{\lambda_o}{\lambda})^2}$. Where E_{opt} , energy gap, (n_o) , static refractive index, ϵ_∞ , (λ_o) , wavelength, and (S_o) strength of the oscillator. Table 2 lists these characteristics.

The refractive index (linear and non-linear) is shown in Figs. 14 and 15 [43–48]. E_{opt}^{dir} , and E_{opt}^{indir} resulting in a minor deviation in the (n_D) . Furthermore, the dielectric and the static dielectric constant (ϵ_o) , and (ϵ_∞) were determined as: $\epsilon_o = -33$.

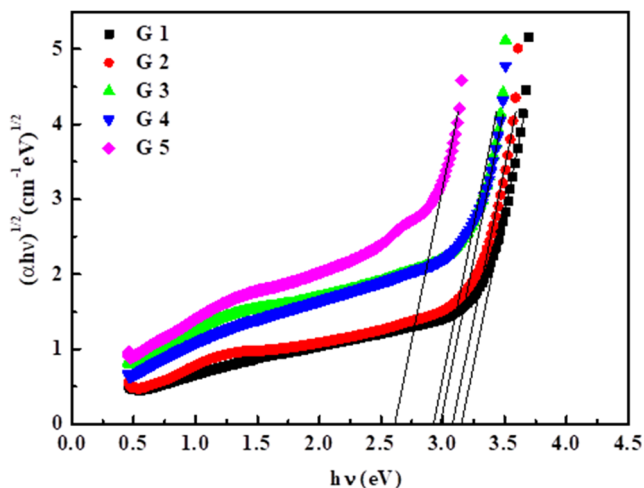


Fig. 6 $(\alpha h\nu)^{1/2}$ versus $(h\nu)$, for $22\text{SiO}_2\text{-}23\text{Bi}_2\text{O}_3\text{-}37\text{B}_2\text{O}_3\text{-}13\text{TiO}_2\text{-(}5-x\text{) LiF-x BaO}$ glasses

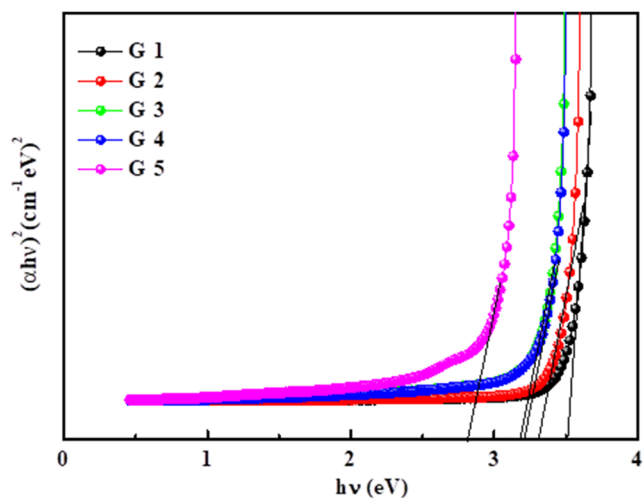


Fig. 7 $(\alpha h\nu)^2$ versus $(h\nu)$, for $22\text{SiO}_2\text{-}23\text{Bi}_2\text{O}_3\text{-}37\text{B}_2\text{O}_3\text{-}13\text{TiO}_2\text{-(}5-x\text{) LiF-x BaO}$ glasses

$26876 + 78.61805E_g - 45.70795E_g^2 + 8.32449E_g^3$, $\epsilon_\infty = n_{AV}^2$. Tables 3 and 4 show the effects of E_{opt}^{dir} , and E_{opt}^{indir} on various optical constrictions. (ϵ_∞) , (ϵ_o) , $\chi^{(1)}$, $(\chi^{(3)})$ and (n_2) .

3.3 DTA Investigation

We used a differential thermal analyzer to investigate the glass's thermal stability [49–55]. In DTA, the glass transition temperature (T_g), crystallization temperature (T_c), and (T_p) are all crucial. T_g which is defined as the temperature range in which a solid material's behavior changes from solid to liquid. T_c is the temperature at which the viscosity of the glass is low enough to prevent rapid crystal growth. T_p is the temperature at which glass crystal formation occurs. The value of $(T_c - T_g)$ has been used to determine the samples' thermal stability (ΔT), so it is preferable to have a large value for $(T_c - T_g)$ [49–55]. For $22\text{SiO}_2\text{-}23\text{Bi}_2\text{O}_3\text{-}37\text{B}_2\text{O}_3\text{-}13\text{TiO}_2\text{-(}5-x\text{) LiF-x BaO}$ glasses

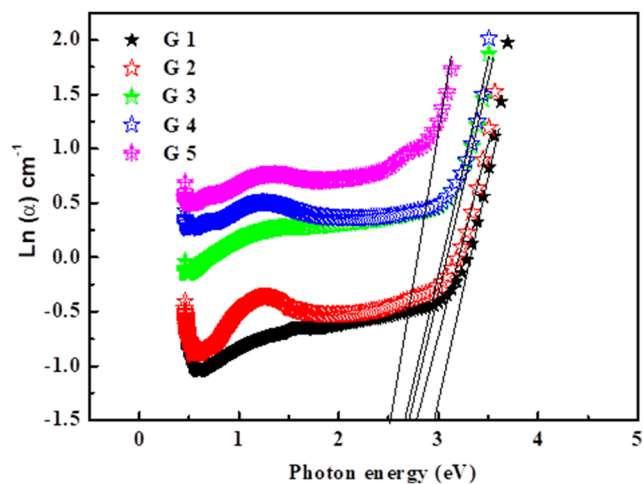


Fig. 8 $\ln(\alpha)$ versus $(h\nu)$, for $22\text{SiO}_2\text{-}23\text{Bi}_2\text{O}_3\text{-}37\text{B}_2\text{O}_3\text{-}13\text{TiO}_2\text{-(}5-x\text{) LiF-x BaO}$ glasses

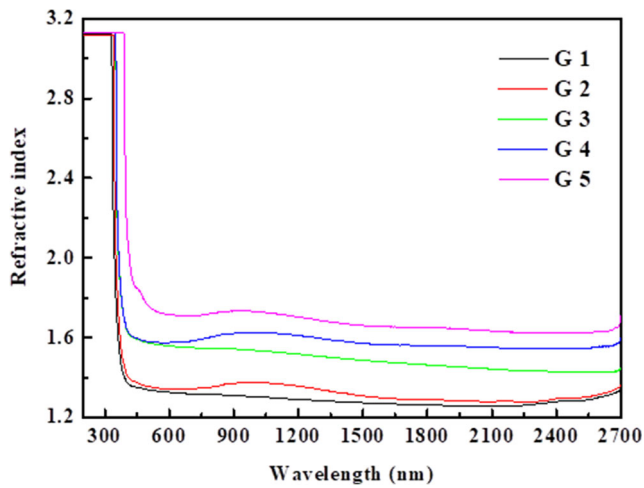


Fig. 9 n_D for $22\text{SiO}_2\text{-}23\text{Bi}_2\text{O}_3\text{-}37\text{B}_2\text{O}_3\text{-}13\text{TiO}_2\text{-}(5-x)\text{LiF-x BaO}$ glasses

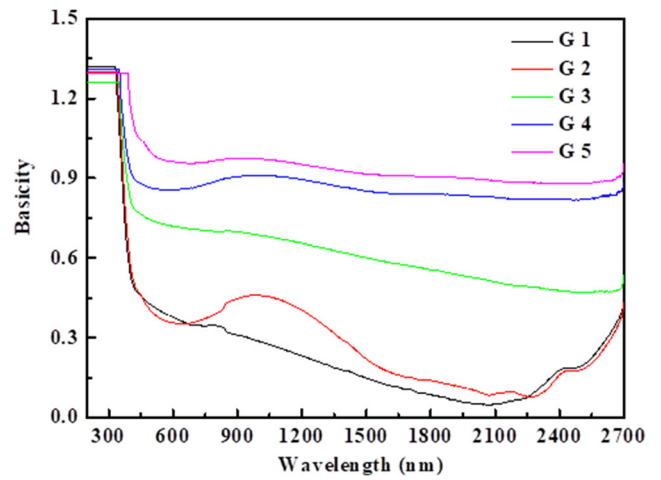


Fig. 12 for $22\text{SiO}_2\text{-}23\text{Bi}_2\text{O}_3\text{-}37\text{B}_2\text{O}_3\text{-}13\text{TiO}_2\text{-}(5-x)\text{LiF-x BaO}$ glasses

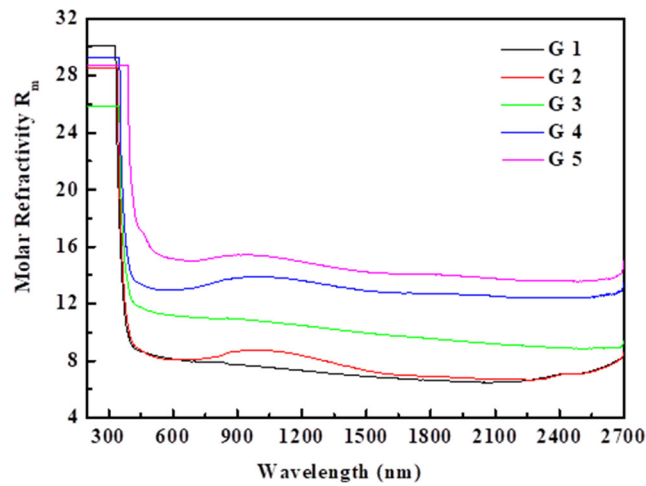


Fig. 10 R_m for $22\text{SiO}_2\text{-}23\text{Bi}_2\text{O}_3\text{-}37\text{B}_2\text{O}_3\text{-}13\text{TiO}_2\text{-}(5-x)\text{LiF-x BaO}$ glasses

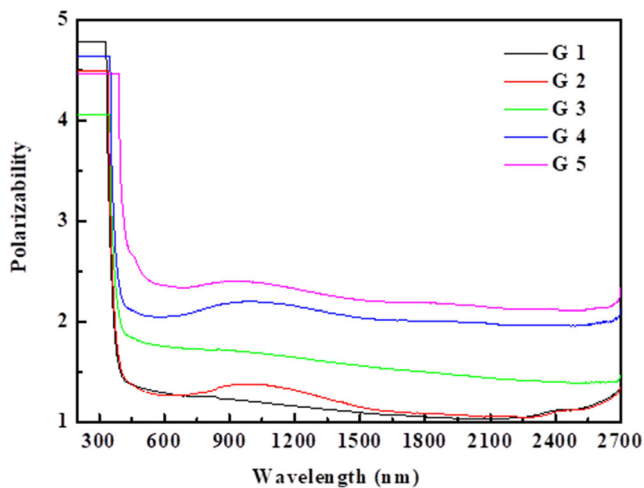


Fig. 11 α_0^{2-} for $22\text{SiO}_2\text{-}23\text{Bi}_2\text{O}_3\text{-}37\text{B}_2\text{O}_3\text{-}13\text{TiO}_2\text{-}(5-x)\text{LiF-x BaO}$ glasses

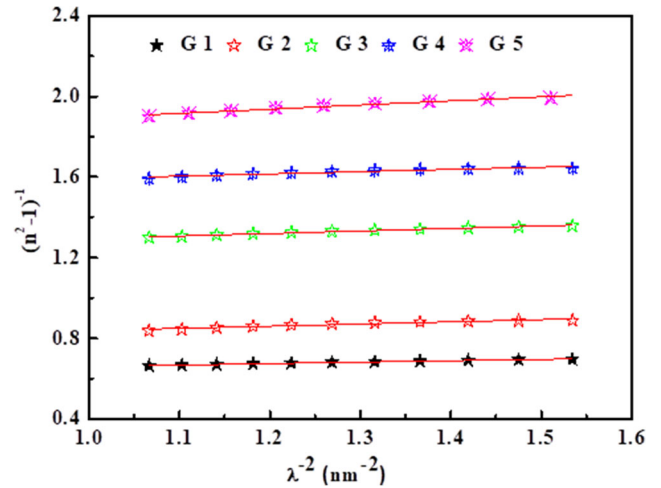


Fig. 13 $(n^2 - 1)^{-1}$ versus λ^{-2} for $22\text{SiO}_2\text{-}23\text{Bi}_2\text{O}_3\text{-}37\text{B}_2\text{O}_3\text{-}13\text{TiO}_2\text{-}(5-x)\text{LiF-x BaO}$ glasses

Table 2 $E_0, E_d, E_{opt}, n_0, \epsilon_\infty, (\lambda_0)$, and (S_0) values of $22\text{SiO}_2\text{-}23\text{Bi}_2\text{O}_3\text{-}37\text{B}_2\text{O}_3\text{-}13\text{TiO}_2\text{-}(5-x)\text{LiF-x BaO}$

Sample	E_0	E_d	E_{opt} (eV)	n_0	ϵ_∞	S_0 (m^{-2})	λ_0 (nm)
G 1	2.47	3.67	1.83	1.576	2.48	1.956	413.97
G 2	2.6	3.06	1.53	1.473	2.17	2.06	477.33
G 3	4.92	2.90	1.45	1.261	1.59	2.03	504
G 4	1.70	2.87	1.44	1.640	2.7	1.986	534.5
G 5	3.54	2.58	1.29	1.315	1.73	2	569.7

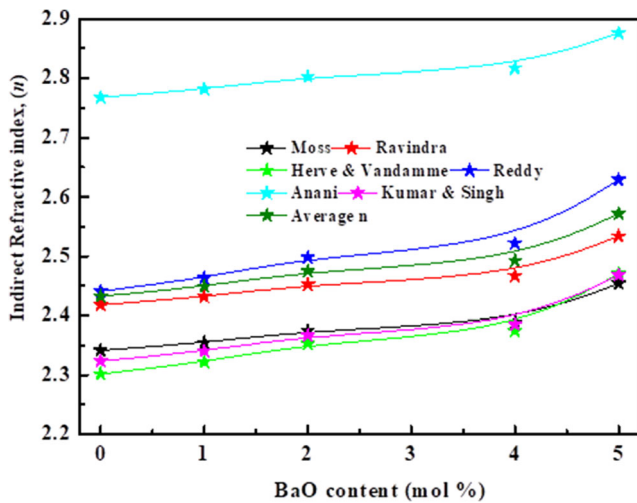


Fig. 14 Non-linear n_D for $22\text{SiO}_2\text{-}23\text{Bi}_2\text{O}_3\text{-}37\text{B}_2\text{O}_3\text{-}13\text{TiO}_2\text{-(}5-x\text{) LiF-}x\text{ BaO}$ glasses

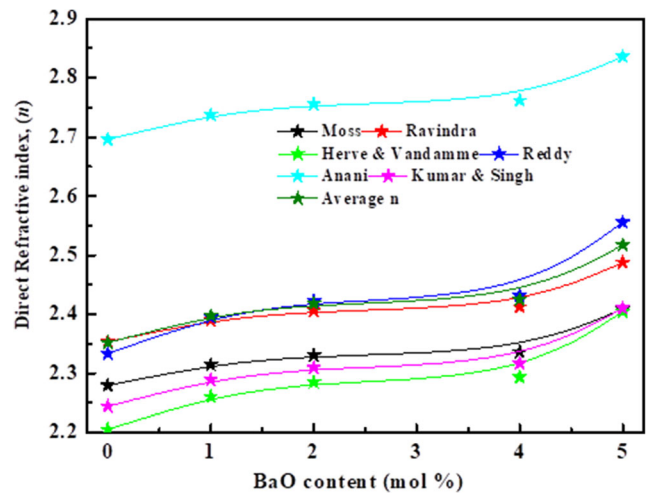


Fig. 15 Linear n_D for $22\text{SiO}_2\text{-}23\text{Bi}_2\text{O}_3\text{-}37\text{B}_2\text{O}_3\text{-}13\text{TiO}_2\text{-(}5-x\text{) LiF-}x\text{ BaO}$ glasses

x BaO glasses, typical DTA traces are shown in Fig. 16. Table 5 lists DTA values of $22\text{SiO}_2\text{-}23\text{Bi}_2\text{O}_3\text{-}37\text{B}_2\text{O}_3\text{-}13\text{TiO}_2\text{-(}5-x\text{) LiF-}x\text{ BaO}$ glasses.

The resistance to a permanent change in characteristics directly impacted by heat is defined as $\Delta T = (T_c - T_g)$. The resistance of glass to crystallization during heating is referred to as glass stability. The creation of bridging oxygens (BO) increases ΔT (from 123 to 137 °C) as BaO increases, as presented in Table 5. Thermally stable glasses have a $\Delta T >$

100 °C. This indicates that the $22\text{SiO}_2\text{-}23\text{Bi}_2\text{O}_3\text{-}37\text{B}_2\text{O}_3\text{-}13\text{TiO}_2\text{-(}5-x\text{) LiF-}x\text{ BaO}$ glasses can be heated above T_g without crystallizing. Thermodynamic stability is also measured by other criteria [56], weighted thermal stability $H_g = \frac{T}{T_g}$. As presented in Table 5 H_g increased (from 0.34 to 0.35 °C), these behaviors indicated that the $22\text{SiO}_2\text{-}23\text{Bi}_2\text{O}_3\text{-}37\text{B}_2\text{O}_3\text{-}13\text{TiO}_2\text{-(}5-x\text{) LiF-}x\text{ BaO}$ glasses Thermally stable.

T_g increased (from 360 to 390 °C), T_c increased (from 483 to 527 °C), and T_p increased (from 593 to 618 °C) in the

Table 3 (ϵ_∞), (ϵ_0), $\chi^{(1)}$, ($\chi^{(3)}$) and (n_2) value as a function of E_{opt}^{indir} .

Sample name	dielectric constant		Nonlinear parameters			F	β absorption coefficient
	ϵ_∞	ϵ_0	$\chi^{(1)}$ (esu)	$\chi^{(3)}$ 10^{-12} (esu)	(n_2) 10^{-11} (esu)	F	β
G 1	5.92	21.42	0.39	3.99	6.18	0.03125	2.378
G 2	5.998	18.84	0.398	4.26	6.5	0.03125	2.509
G 3	6.12	15.54	0.408	4.71	7.17	0.03125	2.73
G 4	6.2	13.7	0.415	5.04	7.62	0.03125	2.88
G 5	6.61	8.67	0.447	6.79	9.94	0.03125	3.7

Table 4 (ϵ_∞), (ϵ_0), $\chi^{(1)}$, ($\chi^{(3)}$) and (n_2) value as a function of E_{opt}^{dir} .

Sample name	dielectric constant		Nonlinear parameters			F	β absorption coefficient
	ϵ_∞	ϵ_0	F	β	(n_2) 10^{-11} (esu)	F	β
G 1	5.53	40.19	0.36	2.88	4.61	0.03125	1.84
G 2	5.75	28.06	0.378	3.48	5.46	0.03125	2.13
G 3	5.85	23.88	0.386	3.77	5.88	0.03125	2.274
G 4	5.88	22.62	0.389	3.88	6.03	0.03125	2.325
G 5	6.34	11.63	0.425	5.54	8.29	0.03125	3.124

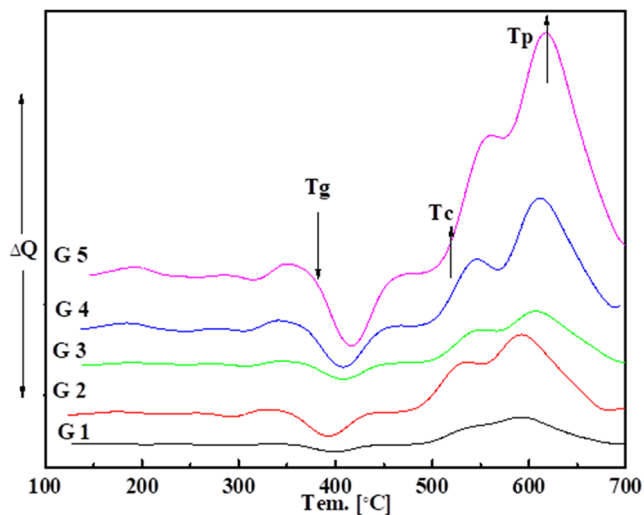


Fig. 16 DTA of $22\text{SiO}_2\text{-}23\text{Bi}_2\text{O}_3\text{-}37\text{B}_2\text{O}_3\text{-}13\text{TiO}_2\text{-}(5-x)\text{LiF-x BaO}$ glasses

current study. It is well known that changes in glass structure affect in (T_g), and ΔT of glasses is visible in close-packed structures. In the current study, LiF was substituted for BaO because single-bond Ba–O energy in the glass network is higher than Li–F energy, making these glasses more stable. Moreover, BaO has a higher average cross-link density than LiF, which contributes to its superiority. Figure 17 presented DTA of values of $22\text{SiO}_2\text{-}23\text{Bi}_2\text{O}_3\text{-}37\text{B}_2\text{O}_3\text{-}13\text{TiO}_2\text{-}(5-x)\text{LiF-x BaO}$ glasses with BaO content.

4 Conclusions

Using melt-quenching techniques, the glass system $22\text{SiO}_2\text{-}23\text{Bi}_2\text{O}_3\text{-}37\text{B}_2\text{O}_3\text{-}13\text{TiO}_2\text{-}(5-x)\text{LiF-x BaO}$ was prepared. The influences of BaO on the thermal and optical characteristics of fabricated glasses were investigated in the current article. The fabricated samples are amorphous, according to XRD analysis. In this manuscript, the molar volume is reduced while the density is raised. The thermal stability of fabricated glasses is mainly affected by changes in glass network connectivity. In the current study, LiF was substituted for BaO because

Table 5 DTA of values of $22\text{SiO}_2\text{-}23\text{Bi}_2\text{O}_3\text{-}37\text{B}_2\text{O}_3\text{-}13\text{TiO}_2\text{-}(5-x)\text{LiF-x BaO}$ glasses ($^{\circ}\text{C}$)

Sample name	T_g	T_c	T_p	ΔT	H_g
G 1	360	483	593	123	0.34
G 2	364	489	597	125	0.34
G 3	372	503	607	131	0.35
G 4	381	515	611	134	0.35
G 5	390	527	618	137	0.35

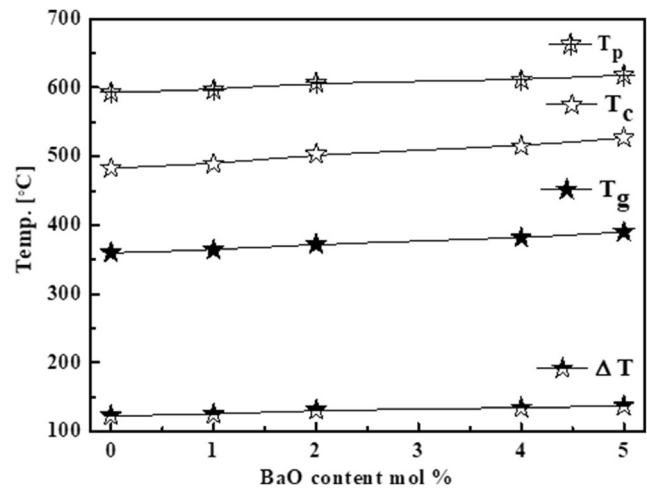


Fig. 17 Parameters of values $22\text{SiO}_2\text{-}23\text{Bi}_2\text{O}_3\text{-}37\text{B}_2\text{O}_3\text{-}13\text{TiO}_2\text{-}(5-x)\text{LiF-x BaO}$

single-bond Ba–O energy in the glass network is higher than Li–F energy, making these glasses more stable. Moreover, BaO has a higher average cross-link density than LiF, which contributes to its superiority. Therefore, as BaO levels rise, all the thermal parameters rise as well. The fabricated glass samples showed a decrease in optical bandgap E_{opt}^{dir} , and E_{opt}^{indir} while (E_u) increased. Molar refractivity, molar polarization, polarizability, and optical basicity all decrease as BaO content rises. Using the Wemple and Didomenico principles, the E_0 , E_d , E_{opt} , n_o , ϵ_{∞} , (λ_o), and (S_o) dispersion parameters were determined.

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