



Chemical Composition, Mechanical, and Thermal Characteristics of Bioactive Glass for Better Processing Features

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Received: 27 December 2021 / Accepted: 17 February 2022 / Published online: 19 March 2022
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Abstract

Glass system was designed using the formula $34\text{B}_2\text{O}_3 - 9\text{SiO}_2 - 18\text{CaO} - 14\text{P}_2\text{O}_5 - (25 - x)\text{Na}_2\text{O} - x\text{TiO}_2$, $x = (0 \leq x \leq 5 \text{ mol}\%)$ in this article. Glass systems were investigated in terms of physical, structural, thermal, and mechanical characteristics. Furthermore, XRD was used to characterize amorphous nature systematically. The structural networks in the samples were analyzed by FTIR spectra to illustrate structural units like SiO_4 , TiO_4 , BO_3 , and BO_4 . Titanium ions act as a trigger to convert BO_3 into BO_4 units, according to preliminary FT-IR results. The glass density and velocities increased after adding TiO_2 . The experimental and theoretical elastic moduli increased with increasing glass densities and velocities. The increasing trend of ΔT with increasing TiO_2 concentration suggested that glass stability had enhanced. According to the results of this study, the mechanical and thermal features of the bioactive glass compositions studied are significantly influenced by the addition of TiO_2 . This research could be used in the future to improve the mechanical and thermal efficiency of bioactive glass systems. G 5 is the best one in terms of mechanical and thermal properties according to these findings.

Keywords Bioactive glass · Mechanical · DTA · FT-IR

1 Introduction

Biocompatible materials for implant applications have gotten a lot of attention in recent years [1–7]. In dental prosthetics and orthopedic implants, as a filler material, bioactive glasses are used. The existence of bioactive glasses with a variety of

physicochemical and mechanical characteristics expands the variety of potential therapeutic options. It has been attempted to describe the impacts of thermal treatment conditions and bioactivity [8–12].

45S5 is the most commonly used bioactive glass for many applications [13, 14]. When B_2O_3 is added to 45S5 bioglass, the glass's acellular bioactive behavior improves as a result. Sitarz et al. [15] and his associates used SEM, EDAX, MIR, and NMR procedures to investigate the bioactivity of B_2O_3 mixed $\text{NaCaPO}_4\text{-SiO}_2\text{-PO}_4$ glasses. Several efforts have been made in recent years to modify the chemical composition of bioactive glasses to control the rate of degradation and mechanical strength and incorporate other oxides like Na_2O , CaO , Al_2O_3 , and TiO_2 into the bioactive glass [16–18]. The elastic properties of biomaterials have been measured using various techniques, for instance, ultrasonic procedures. The ultrasonic non-destructive method procedure has long been regarded as a one-of-a-kind tool for determining the properties of materials.

The presence of TiO_2 in glasses has a significant impact on structural, physical, and thermodynamic properties, including polymerization degree [5, 10, 19–30]. Duan et al. [31] & Moghanian et al. [32–41] examined the mechanism

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of TiO₂'s role in the CaO–Al₂O₃–SiO₂–TiO₂ glass structure. Bioglass-based medical products in orthopedics and dentistry are the most common. These glasses have been studied in terms of a variety of factors, including modifying a chemical formulation. Thermal stability and mechanical characteristics were found to increase as the concentration of TiO₂ increased, indicating the formation of oxygen bridges (BO). Herein, we are focusing on the XRD, FT-IR, DTA, and ultrasonic velocities of the glass samples which are not yet widely studied. The relevant information here is used to determine the optimal glass composition for biomedical applications. The high reactivity of these materials is their primary benefit for periodontal repair and bone augmentation.

2 Methods and Materials

Preparation: 34B₂O₃ – 9SiO₂ – 18CaO – 14 P₂O₅ – (25 – x) Na₂O - xTiO₂, x = (0 ≤ x ≤ 5 mol%) glass in Table 1 and ref. [42] was prepared.

XRD& Density measurements: As ref. [42].

FT-IR: A JASCO 430 spectrometer was used to detect FT-IR absorption.

DTA: A Thermal Analyzer (TA-50 Shimadzu, Japan) was utilized to perform differential thermal analysis (DTA). The glass transition, onset crystallization, and fully crystallization temperatures *T_g*, *T_c*, & *T_p* for each glass were determined using the general procedure for determining *T_g*, *T_c*, and *T_p* for each glass.

Mechanical: The Echo - graph (Krautkramer model USM3) was used to make the ultrasonic measurements.

The longitudinal and shear *V_L*&*V_T* velocities were calculated using this method. In addition to the density, the *V_L*&*V_T* were accustomed to calculating elastic moduli.

Longitudinal : $L = \rho v_l^2,$

Transverse, $G = \rho v_t^2,$

Young's : $Y = (1 + \sigma)2G.$

Table 1 Chemical formulation (mol, %)

code	B ₂ O ₃	SiO ₂	CaO	P ₂ O ₅	Na ₂ O	TiO ₂
G 1	34	9	18	14	25	0
G 2	34	9	18	14	24	1
G 3	34	9	18	14	23	2
G 4	34	9	18	14	22	3
G 5	34	9	18	14	20	5

Bulk : $K = L - \left(\frac{4}{3}\right)G.$

Dimensionality $d = \left(\frac{G}{K}\right)^*4.$

Hardness; $H = \frac{(1-2\sigma)Y}{6(1 + \sigma)}.$

Debye, $\theta_D = \frac{h}{k} \left(\frac{9N}{4\pi V_m}\right)^{\frac{1}{3}} M_s.$

Velocity averages $M_s = \frac{1}{3} \left(\frac{\frac{2}{v_t^2}}{\frac{1}{v_l^2}}\right)^{\frac{1}{3}},$

Expansion of the thermal $\alpha_{P=23.2} (v_L=0.57457),$

oxygen's molar volume $V_o = \left(\frac{M}{\rho}\right) \left(\frac{1}{\sum x_i n_i}\right),$

Oxygen packing density $OPD = \left(\frac{1000 C}{V_m}\right) \left(\frac{Mol}{L}\right).$

The acoustic impedance; $Z = v_L \rho.$

Softening temperature : $T_s = \frac{M*(V_l*100)^2}{\sum_i x_i X_i *(50740)^2}$

The dissociation energy (*Gi*) and packing density(*V_i*) are used in the elastic module's theoretical calculations.

(*V_i*) are used. $V_i = \left(\frac{3\pi}{4}\right)NA \left\{ mR^3 + n R_i^3 \right\} \left(\frac{m^3}{mol}\right),$

$Gi = \left(\frac{1}{V_m}\right) \sum_i Gi Xi.$

The ratio of Poisson's, $\sigma = \frac{1}{2} - \left(\frac{1}{7.2 * V_i}\right).$

3 Results and Discussion

3.1 Physical Characteristics

XRD pattern proves that the glasses have an amorphous state [22, 42–48] (Fig. 1). Density (ρ) and molar volume (*V_m*) are used to examine the physical characteristics of glasses. All of the prepared samples' (ρ) and (*V_m*) values are shown in Fig. 2. G 5 has a significantly higher density than the others. The difference in molecular masses and densities between TiO₂ (79.89 g/mol), (4.23 g. cm⁻³) and Na₂O (61.69 g/mol), (2.27 g. cm⁻³) explains the increase in (ρ) with increasing TiO₂ content. Furthermore, the increase in (ρ) denotes that TiO₂ causes the glass structure to become more compact. It has been discovered that the values of (*V_m*) are lower. This may be due to a decrease in interatomic spacing between the glass networks, which causes a decrease in *V_m*. G 5 has a

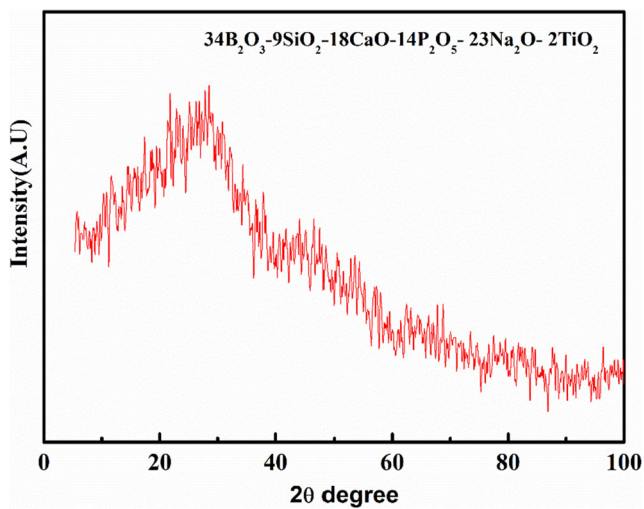


Fig. 1 XRD of $34\text{B}_2\text{O}_3\text{-}9\text{SiO}_2\text{-}18\text{CaO}\text{-}14\text{P}_2\text{O}_5\text{-}23\text{Na}_2\text{O}\text{-}2\text{TiO}_2$ glass sample

significantly lower V_m than the others. The variation in bond length between Ti-Ti (0.2896 nm) and Na₂O (0.3716 nm) explains the decrease in V_m with increasing TiO₂ content [49–56]. As a result, such behavior denotes the presence of BO as a result of TiO₂ substitution. As a result, the values (ρ) and (V_m) of this study agree with the values (ρ) and (V_m) of the calculated El-Maaref et al. [49, 52].

3.2 DTA

The T_g , T_c , & T_p temperatures are parameters that depend on bond strength, cross-link density, and packing density. The relationship between the glass structure and the glass characteristics is reflected in these temperatures [11, 57, 58]. The constructional dependence on TiO₂ amount in the $34\text{B}_2\text{O}_3\text{-}9\text{SiO}_2\text{-}18\text{CaO}\text{-}14\text{P}_2\text{O}_5\text{-}(25-x)\text{Na}_2\text{O}\text{-}x\text{TiO}_2$, $x = (0 \leq x \leq 5 \text{ mol}\%)$ glasses is the most noticeable feature. The DTA profile for all of the samples is shown in Fig. 3 & Table 2. It can be seen in Table 2 that the T_g , T_c , & T_p increases as the

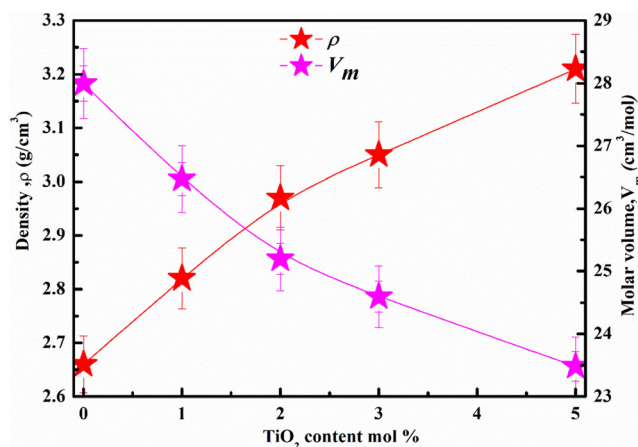


Fig. 2 ρ & V_m of synthetic samples

Table 2 DTA data of investigated glasses

code	T_p (K)	T_g (K)	ΔT	T_c (K)	S	H_g
G 1	951.15	727.15	224	860.15	28.03	0.308
G 2	983.15	748.15	235	889.15	29.53	0.314
G 3	1008.15	754.15	254	909.15	33.34	0.337
G 4	1018.15	771.15	247	924.15	30.11	0.32
G 5	1052.15	788.15	264	950.15	34.17	0.335

TiO₂ content rises. We expose all evidence that validates our description in this work to test the dependence T_g , T_c , & T_p has on other parameters. Because the bond strength of Ti-O (73kcal) is higher than that of Na-O (20 kcal), the T_g , T_c , & T_p values increases with TiO₂.

The thermal stability of the glasses ($\Delta T = T_c - T_g$), weighted thermal stability $H_g = \frac{\Delta T}{T_g}$, S criterion $S = (T_p - T_c) \frac{\Delta T}{T_g}$. ΔT , H_g , and S values increases as the TiO₂ content increases. The most thermally stable glass is the one with the highest TiO₂ content. The term ΔT specifies the glasses' thermal stability, and we reported that ΔT values rise as TiO₂ content rises. The increasing trend of ΔT with increasing TiO₂ concentration, on the other hand, suggested that glass stability had enhanced. As the replacement of weaker Na-O bonds by stronger Ti-O bonds can be attributed to the increasing glass stability as TiO₂ increases. These results are identical to those obtained from the data in [59–61]. As a result, such behavior denotes the presence of BO as a result of TiO₂ substitution. As a result, the values T_g , T_c , & T_p , ΔT , H_g & S of this study agree with the values calculated by Alrowaili et al. & Wahab et al. [52, 59].

We calculated the (OPD) to study the effect of TiO₂ content on T_g , as shown in Table 2, and Fig. 4. The increase in T_g could be explained by the (OPD) parameter, as shown in

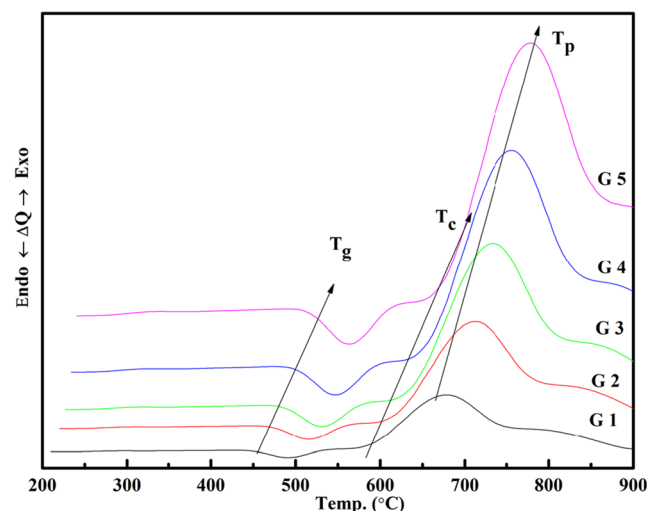


Fig. 3 DTA of investigated glasses

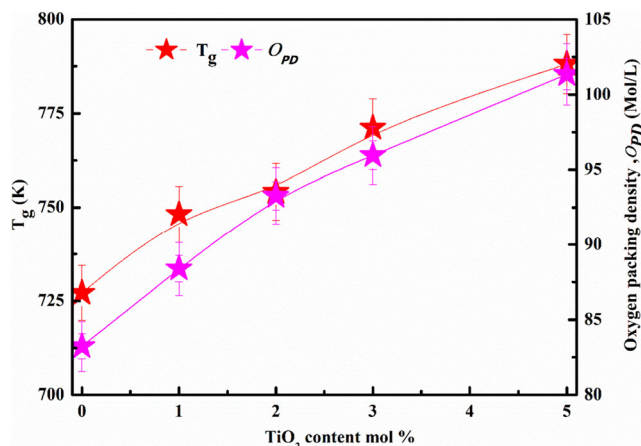


Fig. 4 (O_{BD}) & (T_g) of synthetic samples

Fig. 4. It exhibited a similar trend to that of T_g as TiO_2 content increased. We can deduce that the bond strength and OPD parameters control the variation of T_g based on these two parameters. By forming TiO_x ($x = 4$ or 6), we can link an increase in T_g to an increment in network connectivity. We propose that the titanium structural units in the glass network result in higher connectivity based on the chemical formula $34B_2O_3 - 9SiO_2 - 18CaO - 14 P_2O_5 - (25 - x) Na_2O - xTiO_2$, $x = (0 \leq x \leq 5 \text{ mol}\%)$. As a result, when TiO_2 increases, the T_g value of the glasses increment. The rigidity of the glass network increased as a result of the cross-linking, resulting in an increment in T_g [59–61].

3.3 Mechanical Investigations

Figure 5 and Table 3 present the experimental values of ultrasonic velocities (V_L & V_T) as well as various glass compositions. Table 3 & Fig. 5 show that adding more TiO_2 content increases velocities. V_L values range from 4590 to 5040 m/s, while V_T values range from 2435 to 2610 m/s. With more TiO_2 added, the composition-dependent density increases (V_L & V_T), as shown in Fig. 5. The increase in (V_L & V_T), as TiO_2 content increases, may be due to an increase in bonding oxygen (BO) and, as a result, the glass network's connectivity. Furthermore, the increase in (V_L & V_T), confirm that TiO_2 causes the glass structure to become more compact [51, 62–67]. These results are identical to those obtained from the data in [51, 62–67]. As a result, such behavior denotes the generation of BO with TiO_2 substitution. The values of this study agree with the values calculated by El-Rehim et al., Koubisy et al. & Alothman et al. [62, 63, 65].

With the addition of TiO_2 , all elastic moduli (both experimentally and theoretically) show the same trend of variations across the entire composition range, as shown in Figs. 6, 7 & Table 3. All elastic moduli were an effect by ρ , V_L & V_T . When the Na_2O glass is modified with TiO_2 , the increment

Table 3 Mechanical parameters values

Samples	G 1	G 2	G 3	G 4	G 5
V_L	4590	4705	4820	4895	5040
V_T	2435	2460	2545	2565	2610
L	56.04	62.43	69.00	73.08	81.54
G	15.77	17.07	19.24	20.07	21.87
K	35.01	39.67	43.35	46.33	52.38
Y	41.14	44.77	50.27	52.6	57.59
L_{th}	155.65	173.67	191.76	202.93	226.44
G_{th}	35.58	37.99	40.33	41.85	44.96
K_{th}	108.21	123.02	137.99	147.13	166.49
Y_{th}	91.14	97.90	104.46	108.65	117.23
V_i	0.99	1.05	1.10	1.13	1.19
G_i	10.98	11.15	11.31	11.48	11.81
V_o	12.02	11.31	10.72	10.42	9.87
O_{PD}	83.23	88.40	93.27	95.96	101.36
d	1.80	1.72	1.77	1.73	1.67
T_s	422	432	464	472	491
α_p	106,475	109,143	111,811	113,551	116,915
H	2.06	2.14	2.48	2.53	2.67
M_s	1886.8	1908.1	1972.7	1989.2	2025.7
θ_D	359.4	370.3	389.2	395.6	409.2
Z	1.2	1.3	1.4	1.5	1.6

in elastic moduli is proportional to the increase in sample densities, indicating that Ti ions fill the interstitial positions of the Na glass network [51, 62–67].

As the TiO_2 content increases, the (d), (H), (σ), and (Z) increase as well, reaching a maximum of 5 mol% TiO_2 , as shown in Fig. 8. The glasses under investigation have a (d) parameter of around 2, indicating a two-dimensional structure with growing cross-links. The Poisson's ratio (σ), increases as TiO_2 increases (σ), is the ratio of horizontal to longitudinal strain in a glass system, and it is usually proportional to the

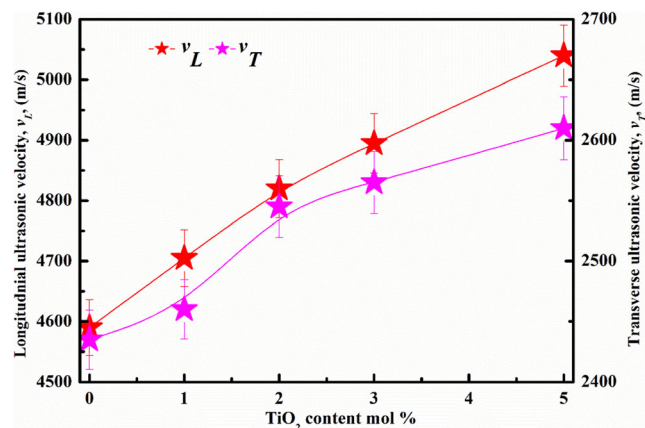


Fig. 5 V_L & V_T of manufactured samples

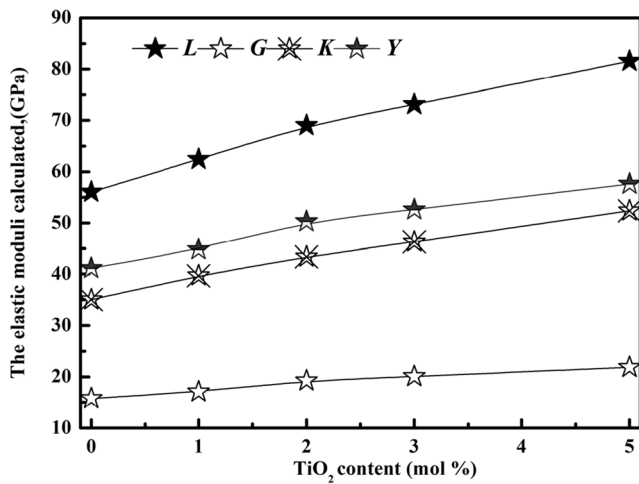


Fig. 6 L, G, K & Y experimentally for glasses

true crosslink density, (σ), increases as the average crosslink density rise. The Debye temperatures (θ_D) and average velocities M_s of TiO₂-containing glass samples are shown in Fig. 9. (θ_D) is dependent on (M_s). As a direct consequence, θ_D increased as TiO₂ content increased. Fig. 10 shows the T_s & α_p for each sample. The addition of TiO₂ enhances T_s & α_p , as previously stated. (V_i) and (G_i) refer to the investigated TiO₂-containing glasses, as shown in Fig. 11. (V_i) and (G_i) values increment as TiO₂ increment [51, 62–67]. These values are illustrated in Table 3. These results are identical to those obtained from the data in [51, 62–67].

3.4 FT-IR Characteristics

The boron in the glasses originated in various vibrational states, as shown in the FT-IR spectra Fig. 12. Furthermore, in many areas of the spectrum, SiO₄ and BO₄ units overlap significantly [3, 4, 21, 45, 68–72]. The bands between 1200

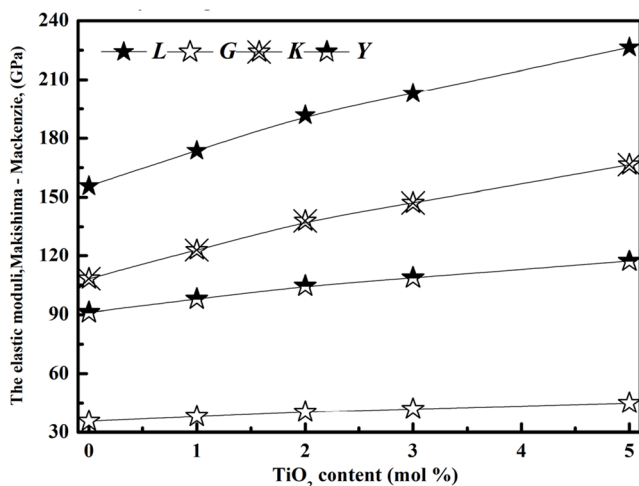


Fig. 7 L, G, K & Y theoretically for glasses

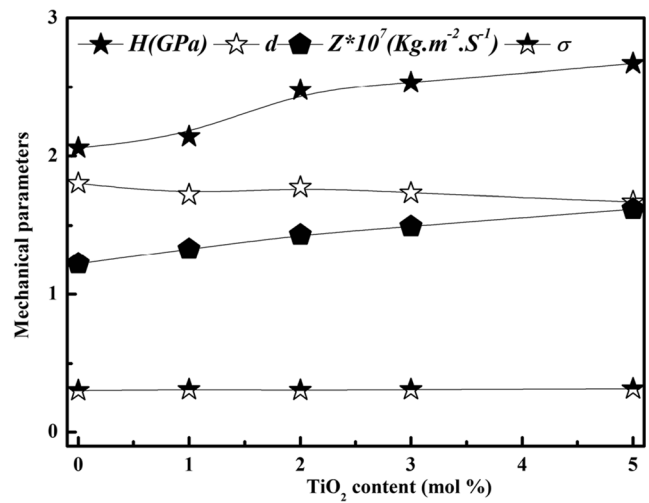


Fig. 8 (d), (H), (σ) & (Z) for glasses

and 1400 cm⁻¹ are related to various (B-O stretching) vibrations, and the absorption at 745 cm⁻¹ belongs to (B-O bending). The presence of BO₄ and BO₃ of boron is represented by these bands. Shoulders amongst 865 cm⁻¹ and 1200 cm⁻¹ on

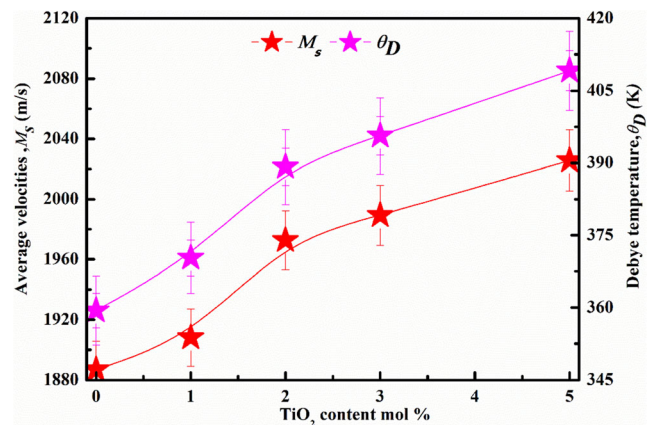


Fig. 9 (θ_D) & (M_s), for glasses

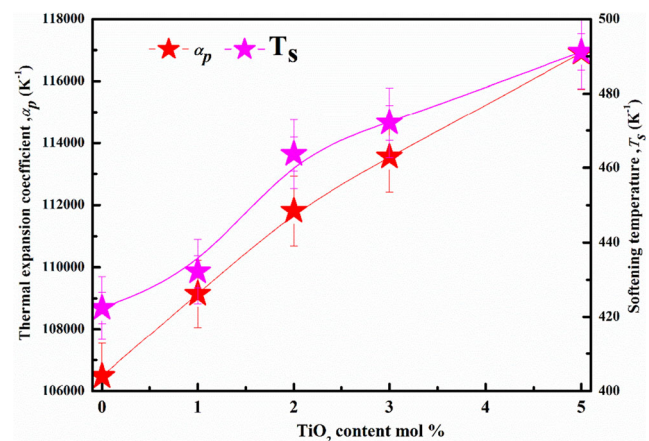


Fig. 10 T_s & α_p for glasses

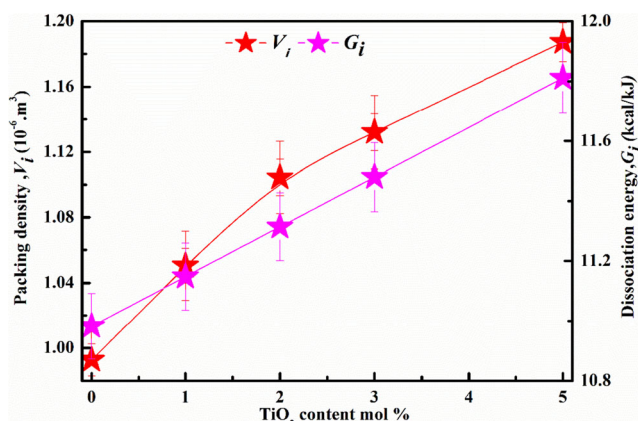


Fig. 11 (V_i) and (G_i) for glasses

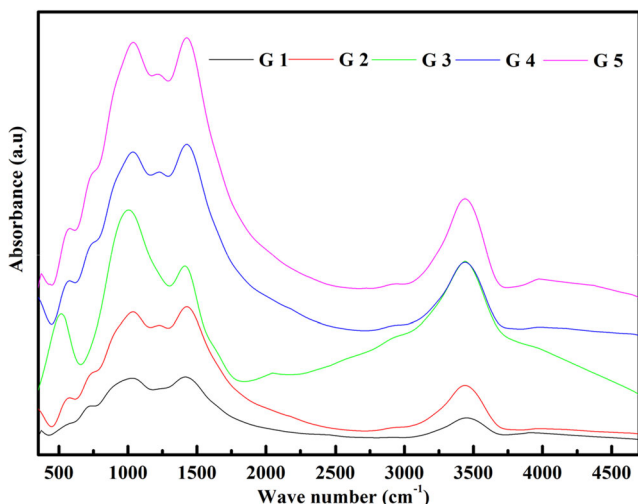


Fig. 12 FT-IR of manufactured samples

the other hand, specify the establishment of BO_4 . However, because of Si-O and P-O bonds. Bands at $374\text{--}392\text{ cm}^{-1}$ due to the vibration of metal cation as Ti^{+2} , Ca^{+2} , & Na^+ . The Si-O-Si bond vibration, which belongs to the (SiO_4) units, is responsible for the band at $442\text{--}405\text{ cm}^{-1}$. The TiO_4 bond vibrations are responsible for the band at $\sim 532\text{ cm}^{-1}$. The (P-O) bond is responsible for the absorption between 570 cm^{-1} .

Furthermore, (Si-O-NBO) bonds can be attributed to the bands in the $1174\text{--}952\text{ cm}^{-1}$ region. Band of 952 cm^{-1} is correlated to O-Ti-O in $[Si(Ti)O_4]$ tetrahedral. Hydrogen bonding is caused by vibrations between $\sim 2887\text{ cm}^{-1}$. H_2O is responsible for the vibrations seen at $\sim 3435\text{ cm}^{-1}$. B can change its coordination number with oxygen from BO_3 to BO_4 , resulting in a variety of anionic environments in which the modifying metal ions can coordinate. The addition of dopants to borosilicate glass makes the structure more stable, which can be deduced.

The effect of titanium ions on the relative of BO_4 and BO_3 was calculated using the deconvolution parameters, such as relative area (A) of FT-IR peaks. The deconvoluted FT-IR spectrum is shown in Fig. 13. For each glass sample, Table 4 lists deconvolution parameters. To calculate the fraction of N_4 & N_3 values, use the following formulas:

$$N_4 = \frac{A1}{A1 + A2}$$

$$N_3 = 1 - N_4$$

The increase in N_4 values correspond to a rise in BO_4 units and the decrease in N_3 values correspond to a reduction in BO_3 units. BO_3 and BO_4 units coexist in the glass composition, according to FT-IR spectra. Titanium ions appear to convert trigonal BO_3 units into tetrahedral BO_4 units, according to preliminary FT-IR results [3, 4, 21, 45, 68–72].

4 Conclusions

The physical, thermal, and mechanical characteristics of glass systems $34B_2O_3 - 9SiO_2 - 18CaO - 14 P_2O_5 - (25 - x) Na_2O - xTiO_2$, $x = (0 \leq x \leq 5\text{ mol}\%)$ were investigated. The absence of peaks in the XRD spectra signifies the amorphous phase of the fabricated samples. The structural network in the samples was confirmed by FTIR spectra to contain structural units like SiO_4 , TiO_4 , BO_3 , and BO_4 . Titanium ions appear to

Table 4 Deconvolution parameters of the glasses under investigation

Glass	Component	Peak (cm ⁻¹)	Area (A)	Area (A2)	N_4	N_3									
G 1	C	374	—	570	713	869	986	1072	—	1210	1410	(A1)	(A2)	N_4	N_3
	A	2.79	—	13.35	7.03	23.36	16.57	10.57	—	15.57	10.75	50.504	26.323	0.657	0.343
G 2	C	—	405	559	721	868	966	1055	—	1206	1413	—	—	—	—
	A	—	3.01	10.49	13.98	17.35	17.32	14.84	—	14.69	8.31	49.507	23.009	0.683	0.317
G 3	C	—	442	532	745	883	992	1081	—	1235	1418	—	—	—	—
	A	—	9.37	10.46	8.31	13.78	20.81	15.38	—	13.50	8.39	49.973	21.891	0.695	0.305
G 4	C	392	—	558	720	885	—	1035	1132	1235	1410	—	—	—	—
	A	4.50	—	8.58	14.10	17.71	—	23.79	12.64	9.21	9.48	54.132	18.687	0.743	0.257
G 5	C	378	—	567	729	864	952	1045	1174	—	1419	63.257	7.394	0.895	0.105
	A	2.90	—	12.29	14.17	11.97	12.88	10.42	27.98	—	7.39	—	—	—	—

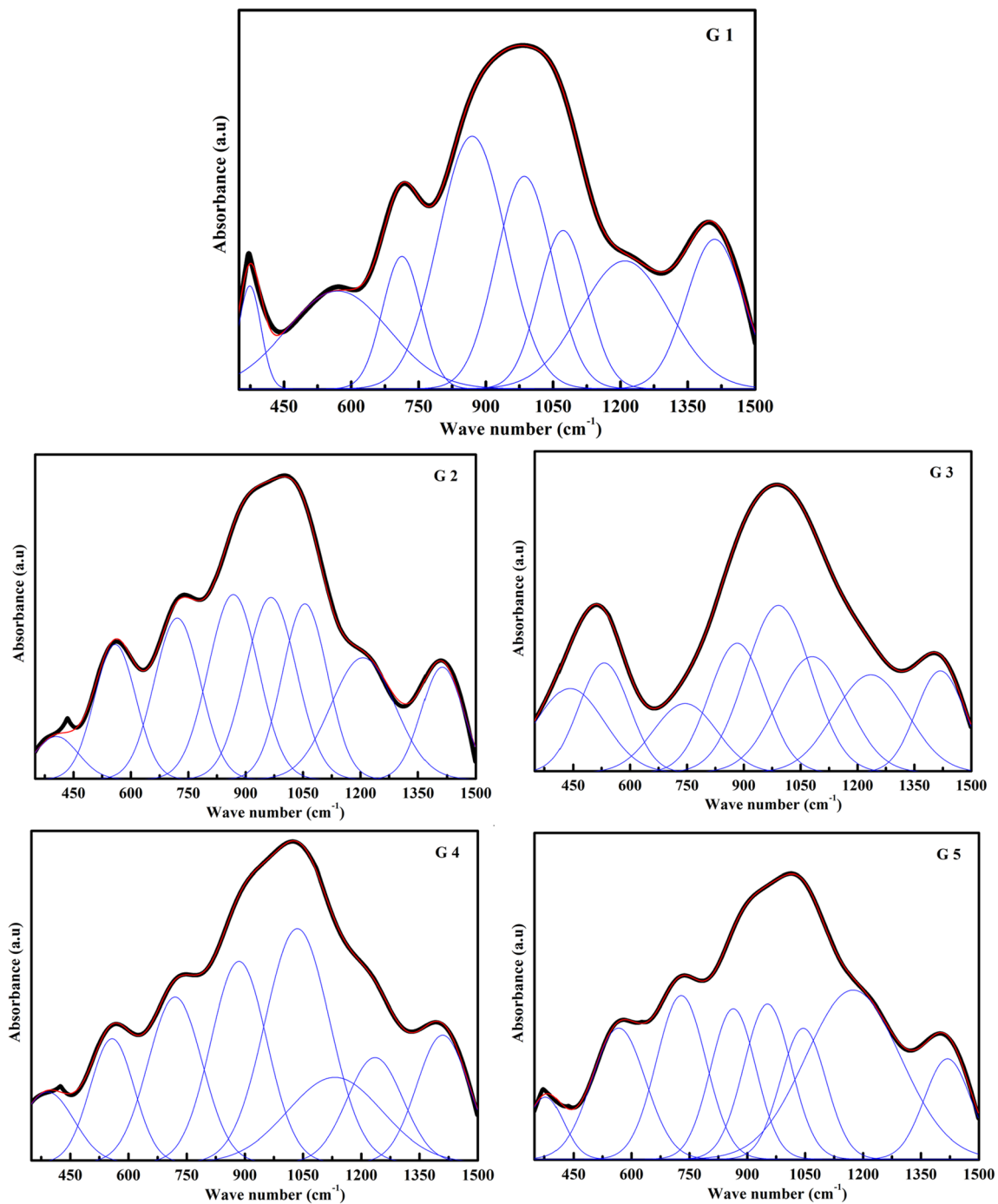


Fig. 13 De-convoluted FT-IR spectrum

convert BO_3 into BO_4 units, according to preliminary FT-IR results. The glass density and velocities increased after TiO_2 was added. The experimental and theoretical elastic moduli increase with increasing glass densities and velocities. The increasing trend of ΔT with increasing TiO_2 concentration suggested that glass stability had enhanced. According to the results of this study, the mechanical and thermal properties of the bioactive glass compositions studied are significantly influenced by the addition of TiO_2 . This research could be used

in the future to enhance the mechanical and thermal efficiency of bioactive glass systems.

Acknowledgments The authors express their gratitude to princess Nourah bint Abdulrahman University, Researchers Supporting Project (Grant No. PNURSP2022R32) Princess Nourah bint Abdulrahman University, Riyadh, Saudi Arabia. Moreover, we would like to thank Taif University Researchers Supporting Project number (TURSP-2020/250), Taif University, Taif, Saudi Arabia.

Author Contributions All of the authors have taken full responsibility for the content of this manuscript.

Data Availability My manuscript and associated personal data.

Compliance with Ethical Standards The manuscript has not been published elsewhere.

Conflict of Interest The authors declare that they have no conflict of interest.

Declaration of Competing Interest There are no known competing financial interests among the authors.

Consent to Participate & Publication The author's consent to participate & publication.

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