

# Effect of TiO<sub>2</sub>/V<sub>2</sub>O<sub>5</sub> substitution on the optical and radiation shielding properties of alkali borate glasses: A Monte Carlo investigation



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## ABSTRACT

In this paper, we used Geant4 Monte Carlo simulations to investigate the effect of TiO<sub>2</sub>/V<sub>2</sub>O<sub>5</sub> substitution on the radiation shielding properties of alkali borate glasses in the chemical form of 30Li<sub>2</sub>O + 55B<sub>2</sub>O<sub>3</sub> + 5ZnO + xTiO<sub>2</sub> + (10 - x)V<sub>2</sub>O<sub>5</sub>, where x = 0, 2.5, 5, 7.5, and 10 mol%. Also, the optical properties were examined by evaluating several factors such as molar refraction (R<sub>m</sub>), metallization criterion (M), molar polarizability (α<sub>m</sub>), dielectric coefficients (static and optical), optical transmission (T), and reflection loss (R<sub>L</sub>). The radiation shielding properties of the tested glasses were estimated by determining the mass attenuation coefficient, and other related factors such as the tenth value layer (TVL), the mean free path (MFP), the electron total stopping powers (Ψ<sub>e</sub>) and the electron continuous slowing down approximation range (CSDA) (Φ<sub>e</sub>) for different energy values. The results of Geant4 Monte Carlo were compared with the theoretical values calculated by XCOM platform. The results revealed that the TiO<sub>2</sub>/V<sub>2</sub>O<sub>5</sub> substitution had a remarkable influence on the gamma shielding properties for the tested glasses. On the other hand, the optical properties slightly changed by the TiO<sub>2</sub>/V<sub>2</sub>O<sub>5</sub> substitution. The gamma shielding properties of the tested glasses were compared with many samples in terms of MFP. The present glasses showed superior features to apply for optical and radiation shielding applications.

## 1. Introduction

Nowadays, glasses are being utilized in numerous technological fields such as photonic field, medical field, industrial field, telecommunication field and other recent fields. In photonic field, glasses are used in optical fiber, optical switching, optical insulators, laser amplifier, optical power limiters and fiber Bragg gratings [1–4]. Glasses are used in the medical field in several ways, where one of the most common applications of the glasses in this field is the bioactive glasses. Bioactive glasses is utilized to fit the needs of different dental as well as medical applications, such as bone grafting and tissue engineering [5]. Also, glasses are used in manufacturing the laboratory flasks, laboratory beakers and microscopic slide. The most important applications of the glasses are the X-ray shielding glass. The purpose of the X-ray glass is to protect people who utilizing radioisotopes or diagnostic imaging

windows from radiation, at the same time providing a clear view. In addition, it provides protection for medical staff when performing radiology, fluoroscopy, mammographies and CT scans [6–8]. The X-ray and Gamma ray are photons which carry adequate energy and can ionize the medium that pass through and accordingly both types of radiation are called ionizing radiation. The ionizing radiation is mostly harmful and potentially sufficient to cause death to the peoples. For this reason, scientists are focus in the last few years to find a convenient method to reduce the exposed dose by utilizing special types of medium known as protection/shielding materials [9–11]. The expression "shielding" is fundamentally based on the fact that some medium has an ability to reduce the influence of radiation by several processes namely scattering, absorption, etc. The radiation shielding ability of the medium affects by the thickness of the medium, its density and the energy of radiation. Practically, lead is a popular material utilized for shielding

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**Table 1**

Glass code, compositions in mol%, percentages by weight (wt%) of elements and densities of the  $30\text{Li}_2\text{O}-55\text{B}_2\text{O}_3-5\text{ZnO}-x\text{TiO}_2-(10-x)\text{V}_2\text{O}_5$ , ( $0 \leq x \leq 10$ ) glasses.

Label	Composition in mol %					Density (g/cm <sup>3</sup> )
	Li <sub>2</sub> O	B <sub>2</sub> O <sub>3</sub>	ZnO	TiO <sub>2</sub>	V <sub>2</sub> O <sub>5</sub>	
LBZ-TV1	30	55	5	–	10	2.610
LBZ-TV2	30	55	5	2.5	7.5	2.570
LBZ-TV3	30	55	5	5	5	2.540
LBZ-TV4	30	55	5	7.5	2.5	2.530
LBZ-TV5	30	55	5	10	–	2.520

goals to protect people or object from radiation and to decrease the effective dose [12]. However, lead has several disadvantages where the most important point in this regard is the toxicity of the lead. Therefore, the use of lead in the shielding field becomes critical issue due to its unhealthy nature. So, it is important to find cheap, safe and nontoxic alternative materials for radiation shielding goals [13].

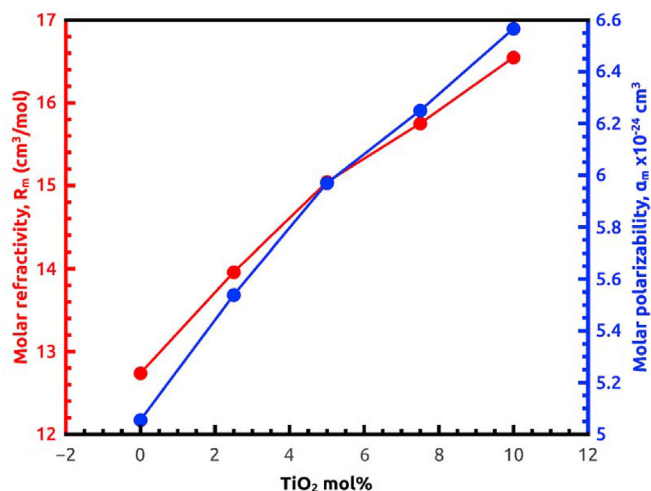
Glasses have a noteworthy attention from radiation protection developers since they have less toxicity from lead and can prepare easily with different fabrications techniques. Also, glasses have good optical transparency and this is important for utilizing the glasses in several optical applications. Moreover, the density of the glass can be changed easily and at a minimal cost by using some heavy metal oxides, thus improving the shielding properties of the proposed glass in the practical applications [14–16]. Among several glass systems, borate glasses have aroused widespread interest in different technological applications due to several interesting physical features [17–19]. In recent years, researchers have started to take advantage of the interesting features of the borate glasses to develop new protective materials from gamma rays [20–22]. In the radiation shielding field, investigators can estimate the radiation attenuation features of any medium using several ways, where the experimental method is the most convenient way to estimate exactly the ability of the medium to shield the photons and thus to draw a conclusion about the effectiveness of the medium to use as shielding material [23]. Due to some special circumstances such as the lack of radioisotopes and equipment which necessary to conduct experiments, or due to some environmental and health conditions such as the closure of universities and research centers due to the spread of coronavirus disease (COVID-19), researchers resort to alternative methods of conducting experiments in the laboratory to test the properties of radiation shielding for different materials. One of the most important way in this regard and considered an effective and alternative way to the experimental method is the Monte Carlo simulation [24,25].

In the present work, we used Geant4 Monte Carlo simulations to investigate the radiation shielding competence of  $30\text{Li}_2\text{O} + 55\text{B}_2\text{O}_3 + 5\text{ZnO} + x\text{TiO}_2 + (10-x)\text{V}_2\text{O}_5$  glasses, where  $x = 0, 2.5, 5, 7.5$ , and  $10$  mol%. Moreover, the optical properties of the tested glasses were studied. The results of Geant4 Monte Carlo were compared with the theoretical calculations performed by XCOM platform. The effect of  $\text{TiO}_2/\text{V}_2\text{O}_5$  substitution on all of these properties was discussed in

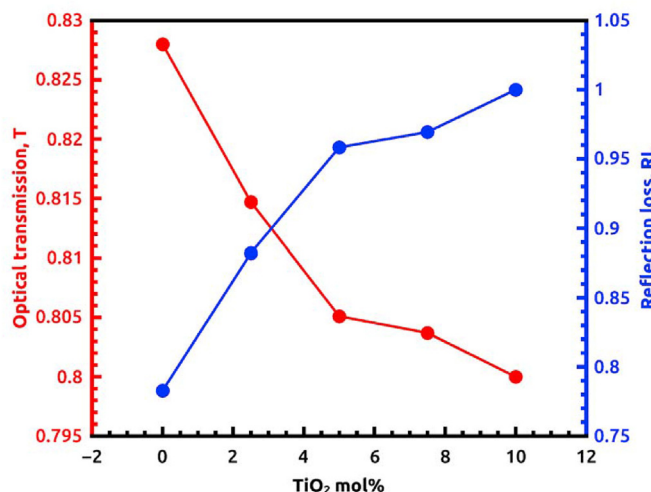
**Table 2**

Optical properties such as  $R_m$ ,  $\alpha_m$ ,  $R_L$ ,  $T$ ,  $M$ ,  $\epsilon^{\text{static}}$ , and  $\epsilon^{\text{optical}}$  of the studied glasses.

Optical property/glass code	LBZ-TV1	LBZ-TV2	LBZ-TV3	LBZ-TV4	LBZ-TV5
Molar volume, $V_m$ (cm <sup>3</sup> /mol)	22.72	24.07	25.36	26.47	27.58
Refractive Index	1.885	1.939	1.979	1.985	2.000
Molar refractivity, $R_m$ (cm <sup>3</sup> /mol)	12.739	13.958	15.043	15.750	16.548
Molar polarizability, $\alpha_m \times 10^{-24}$ cm <sup>3</sup>	5.055	5.539	5.969	6.250	6.567
Reflection loss, $R_L$	0.783	0.882	0.958	0.969	1.000
Optical transmission, $T$	0.828	0.815	0.805	0.804	0.800
Metallization criterion, $M$	0.439	0.420	0.407	0.405	0.400
Static dielectric constant, $\epsilon^{\text{static}}$	3.553	3.761	3.916	3.939	4.000
Optical dielectric constant, $\epsilon^{\text{optical}}$	2.553	2.761	2.916	2.939	3.000



**Fig. 1.** Variation of  $R_m$  and  $\alpha_m$  with the concentration of  $\text{TiO}_2$  mol% for LBZ-TVx glass system.



**Fig. 2.** Variation of optical transmission and reflection loss with the concentration of  $\text{TiO}_2$  mol% for LBZ-TVx glass system.

detail. An extensive comparison was achieved between the gamma shielding properties of LBZ-TVx samples and those of standard gamma shields.

## 2. Materials and methods

The glass samples in the chemical form of  $30\text{Li}_2\text{O} + 55\text{B}_2\text{O}_3 + 5\text{ZnO} + x\text{TiO}_2 + (10-x)\text{V}_2\text{O}_5$ , where  $x = 0, 2.5, 5, 7.5$ , and  $10$  mol%. were prepared as described in Ref. [26]. This glass

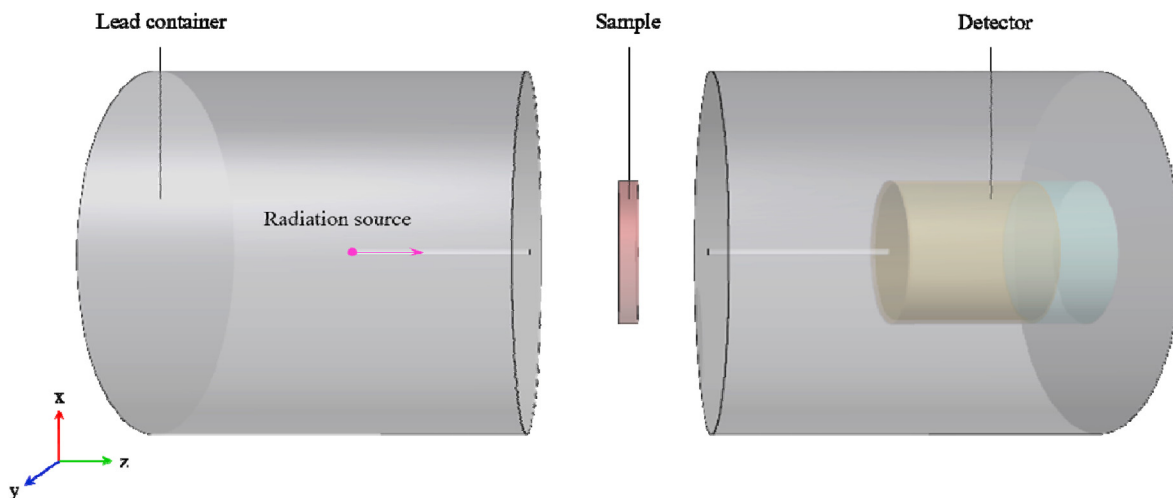


Fig. 3. The geometry of Geant4 simulation.

Table 3

Mass attenuation coefficient ( $\mu/\rho$ ) of the LBZ-TV1, LBZ-TV2, and LBZ-TV3 glasses obtained by Geant4 simulations and XCOM program with different photons energies.

Photon Energy (MeV)	LBZ-TV1			LBZ-TV2			LBZ-TV3		
	XCOM	Geant4	Dev.%	XCOM	Geant4	Dev.%	XCOM	Geant4	Dev.%
0.02	3.9165	3.870	1.18	4.1930	4.118	1.79	4.4476	4.377	1.59
0.04	0.6756	0.663	1.85	0.7118	0.699	1.86	0.7451	0.732	1.77
0.06	0.3139	0.310	1.09	0.3246	0.321	1.17	0.3344	0.332	0.75
0.08	0.2175	0.215	1.32	0.2219	0.220	0.80	0.2260	0.225	0.62
0.1	0.1784	0.176	1.32	0.1806	0.180	0.61	0.1827	0.180	1.44
0.2	0.1231	0.122	1.12	0.1233	0.123	0.63	0.1235	0.122	0.92
0.5	0.0845	0.084	0.93	0.0845	0.084	0.73	0.0844	0.084	1.06
0.8	0.0685	0.068	0.99	0.0684	0.068	1.02	0.0684	0.067	1.34
1	0.0615	0.061	0.67	0.0615	0.061	1.49	0.0614	0.061	1.47
5	0.0272	0.027	0.70	0.0273	0.027	1.00	0.0273	0.027	1.10

Table 4

Mass attenuation coefficient ( $\mu/\rho$ ) of the LBZ-TV4 and LBZ-TV5 glasses obtained by Geant4 simulations and XCOM program with different photons energies.

Photon Energy (MeV)	LBZ-TV4			LBZ-TV5		
	XCOM	Geant4	Dev.%	XCOM	Geant4	Dev.%
0.02	4.6828	4.610	1.55	4.9007	4.809	1.88
0.04	0.7758	0.765	1.37	0.8043	0.791	1.67
0.06	0.3435	0.341	0.67	0.3519	0.348	1.19
0.08	0.2298	0.229	0.52	0.2333	0.232	0.74
0.1	0.1846	0.183	0.71	0.1864	0.184	1.11
0.2	0.1237	0.123	0.79	0.1239	0.123	1.06
0.5	0.0844	0.084	0.82	0.0844	0.083	1.16
0.8	0.0683	0.067	1.21	0.0683	0.068	0.53
1	0.0614	0.061	0.93	0.0613	0.061	0.51
5	0.0274	0.027	0.68	0.0274	0.027	1.18

system was coded as LBZ-TVx according to the ratio of the  $\text{TiO}_2/\text{V}_2\text{O}_5$  substitution. For example the first sample ( $x = 0$ ) is referred by LBZ-TV1. Therefore, we have five glass samples namely; LBZ-TV1, LBZ-TV2, LBZ-TV3, LBZ-TV4, and LBZ-TV5. The densities of these glasses were measured to be 2.610, 2.570, 2.540, 2.530, and 2.520  $\text{g}/\text{cm}^3$  respectively. In the present work, we studied the optical properties of LBZ-TVx glasses. Also, by means of Geant4 code, we identified the gamma shielding properties of the tested samples.

### 2.1. Optical properties

The optical parameters such as  $R_m$ ,  $T$ ,  $R_L$ ,  $\alpha_m$ ,  $\epsilon$  ( $\epsilon^{\text{static}}$  and  $\epsilon^{\text{optical}}$ ),

and  $M$  were evaluated by using the following equations [27,28]:

$$R_m = \left( \frac{n^2 - 1}{n^2 + 2} \right) V_m \text{ and } \alpha_m = \frac{R_m}{2.52} \tag{1}$$

$$T = \frac{2n}{n^2 + 1} \text{ and } R_L = \left( \frac{n - 1}{n + 1} \right)^2 \tag{2}$$

$$\epsilon^{\text{static}} = n^2 \text{ and } \epsilon^{\text{optical}} = \epsilon^{\text{static}} - 1 \tag{3}$$

Finally, the metallization criterion ( $M$ ) parameter can be given by the relation of [28]:

$$M^{\text{criterion}} = 1 - \frac{R^{\text{molar}}}{V_m} \tag{4}$$

### 2.2. Radiation shielding properties

The radiation shielding studies for the tested glasses were carried out by using Monte Carlo method (via Geant4) and some theoretical approaches (via XCOM). Geant4 toolkit is based on C++ language for modeling process of real phenomena, especially those related to high energy physics, medical applications, and radiation transport [29]. Different recent studies used Geant4 to determine the radiation shielding properties for some glass systems [30–35]. In this study, three mandatory classes such as G4RunManager, G4PrimaryGenerator Action, and G4DetectorConstruction were prepared to describe the gamma radiation shielding properties of the studied glasses. We carried out the package of StandardEM to include all the interactions that may be occurred during the passing of radiation through matter. Such

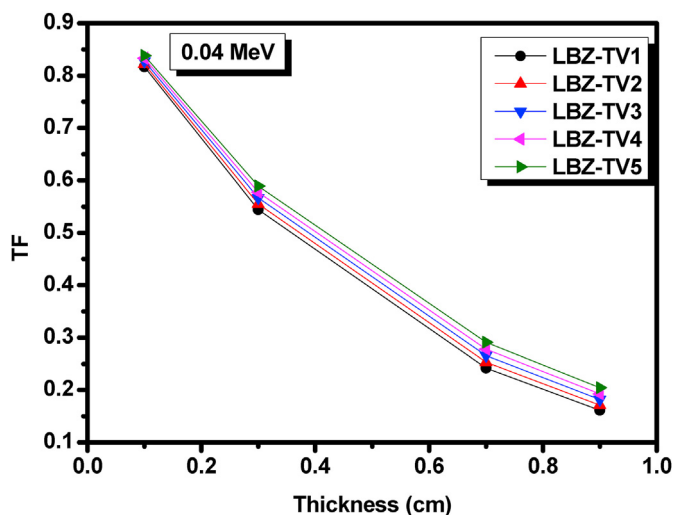


Fig. 4. The transmission factor for the LBZ-TVx glass system as a function of the thickness at 0.04 MeV.

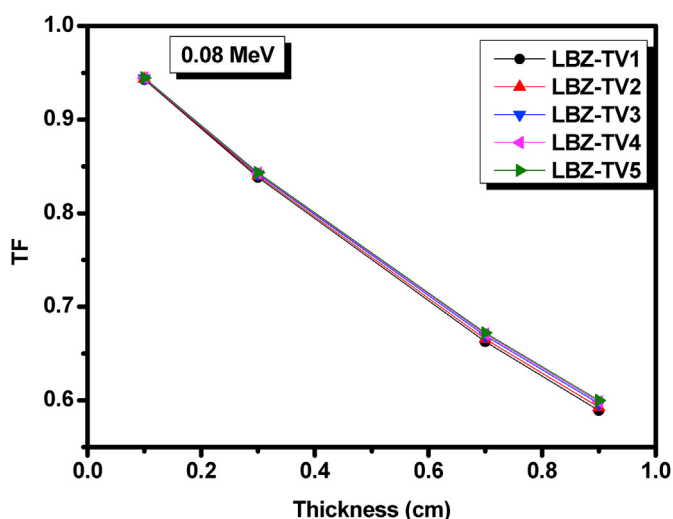


Fig. 5. The transmission factor for the LBZ-TVx glass system as a function of the thickness at 0.08 MeV.

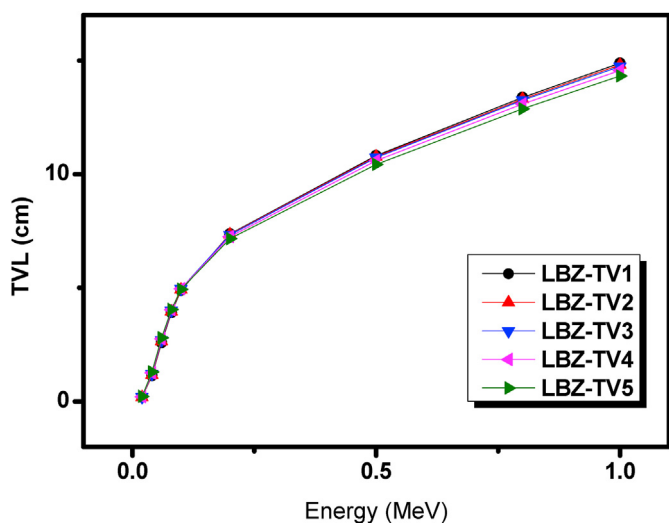


Fig. 6. Tenth value layer (TVL) of LBZ-TVx glass system as function of the photon energy between 0.02 and 1 MeV.

package does not include the nucleus recoil effects and deals with the atomic electrons as quasi free electrons. By using Geant4 simulations, we performed the gamma transmission experiment. One million gamma photons were gunned directly to the studied glasses with thickness of  $x$ , and then the number of passed gamma photons were estimated. By using the numbers of initial and passed photons, we obtained the  $\mu$  that can be easily converted to the  $\mu/\rho$ . This parameter can evaluate the radiation transport of a material. The  $\mu/\rho$  can be also achieved by XCOM program that is based on the following equation [36]:

$$\frac{\mu}{\rho} = \sum_i W_i \left( \frac{\mu}{\rho} \right)_i \tag{5}$$

### 3. Results and discussion

Table 1 shows the sample code, nominal composition, and densities for the LBZ-TVx glasses. According to the  $\text{TiO}_2/\text{V}_2\text{O}_5$  substitution the glass density decreased from  $2.610 \text{ g/cm}^3$  for LBZ-TV1 to  $2.520 \text{ g/cm}^3$  for LBZ-TV5. Such reduction can be explained by two reasons related to the physical properties of  $\text{TiO}_2$  and  $\text{V}_2\text{O}_5$  oxides. The first reason is the density of  $\text{TiO}_2$  ( $4.23 \text{ g/cm}^3$ ) which is bigger than that of  $\text{V}_2\text{O}_5$  ( $3.36 \text{ g/cm}^3$ ). The second reason is the molecular weight of  $\text{TiO}_2$  ( $79.866 \text{ g/mol}$ ) which is smaller than that of  $\text{V}_2\text{O}_5$  ( $181.88 \text{ g/mol}$ ). It is worth mentioning that the density values give a prior information about the optical and the radiation shielding properties of glasses. However, a full understanding of optical and the gamma shielding properties of the glasses needs deep analyze for different parameters as will be discussed below.

The optical features of LBZ-TVx glasses (see Table 2) will be discussed in terms of molar refraction ( $R_m$ ), metallization principle (M), molar polarizability ( $\alpha_m$ ), dielectric coefficients, optical transmission (T), and reflection loss ( $R_L$ ). Fig. 1 shows the variation of  $R_m$  and  $\alpha_m$  as a function of  $\text{TiO}_2$  content. Clearly, there is a direct relation between  $R_m$  and  $\alpha_m$ . The values of  $R_m$  and  $\alpha_m$  increase with the  $\text{TiO}_2/\text{V}_2\text{O}_5$  substitution. Such that the  $R_m$  values were 12.739, 13.958, 15.043, 15.750 and  $16.567 \text{ cm}^3/\text{mol}$  for LBZ-TV1, LBZ-TV2, LBZ-TV3, LBZ-TV4, and LBZ-TV5, respectively. Fig. 2 demonstrates the reflection loss and the optical transmission for the LBZ-TV5 glasses as a function  $\text{TiO}_2$  content. Here, T is inversely with  $R_L$ . At 10 mol% of  $\text{TiO}_2$ , it is found that T is 0.80 and  $R_L$  is 1. All the other optical parameters such as metallization criterion (M), molar polarizability ( $\alpha_m$ ), dielectric coefficients (static and optical), optical transmission (T), and reflection loss ( $R_L$ ) are summarized in Table 2.

The gamma shielding studies were carried out via Geant4 simulation by using the geometry described in Fig. 3. This figure shows the narrow beam geometry containing of radiation source to emit monoenergetic gamma-rays in the range of 20 keV and 5 MeV (we selected 10 energies as given in Table 3 and Table 4). In these two tables, we compared the Geant4 and XCOM in terms of  $\mu/\rho$ . It is evident that the simulated values are close to those of XCOM (especially at lower energy). On the other hand, the differences between two approaches are mainly related to the divergence of the cross section libraries in Monte Carlo method and theoretical calculations. At low photon energies the Geant4 values were observed to be lower than those of XCOM. By increasing the energy, the XCOM values became identical to those of Geant4 [37–42].

For the tested glasses, we calculated the transmission factor ( $\text{TF} = I/I_0$ ), where  $I_0$  and  $I$  are the incident and transmitted photon intensities respectively. We calculated the TF for different glass thicknesses (i.e. 0.1, 0.3, 0.7 and 0.9 cm) and we presented the results at 0.04 MeV in Fig. 4 and at 0.08 MeV in Fig. 5. From these two figures, it is clear that the TF decreases with increasing the thickness of the glass. The TF values for the LBZ-TV1, LBZ-TV2, LBZ-TV3, LBZ-TV4, and LBZ-TV5 glasses at 0.04 MeV are 0.816, 0.822, 0.828, 0.833 and 0.838 (this is for  $x = 0.1 \text{ cm}$ ). For the same glasses but for higher thickness (i.e.

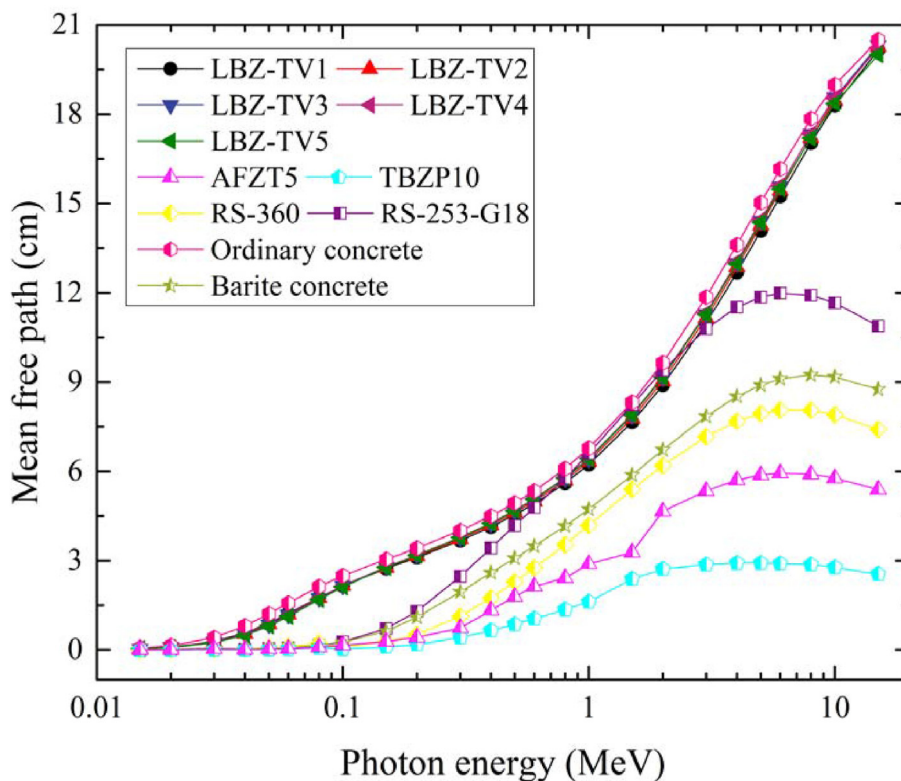


Fig. 7. Variation of mean free path (MFP) with the photon energy for LBZ-TVx glasses in comparison with conventional concrete, HMO glasses, and different commercial glasses.

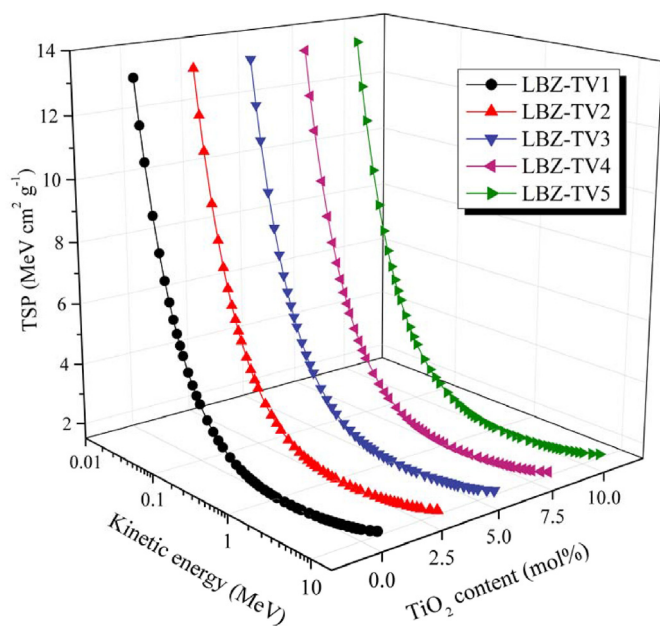


Fig. 8. Variation of electron total stopping powers ( $\Psi_e$ ) as a function of kinetic energy for LBZ-TVx glass system.

$x = 0.7$  cm), the TF values are 0.242, 0.253, 0.266, 0.278 and 0.291 (see Fig. 4). This suggests that increasing the thickness of the selected LBZ-TVx glasses improves the radiation protection features. Also, from Figs. 4 and 5 we found that LBZ-TV1 and LBZ-TV5 have the lowest and highest TF respectively. Moreover, Figs. 4 and 5 reveal that the TF increases with increasing the energy of the photon. For instance, at 0.04 MeV, the TF for LBZ-TV1 with  $x = 0.3$  is 0.544, and this is increased to 0.838 for  $E = 0.08$  MeV.

We also evaluated the tenth value layer (TVL) for the present glasses to directly investigate the gamma ray shielding performance [43,44]. The concept of TVL is utilized to quantify the photon ability in penetrating the glass specimen. The absorber thickness needed to minimize the intensity of a photon to 10% of its original intensity is called as. We determined the TVL for the present glasses for the energy range of 0.02 and 1 MeV and presented the results in Fig. 6.

Considering, Fig. 6, the TVL indicates the thickness required of the glass samples to shield 10% of the original radiation. TVL thickness is beneficial for radiation shielding as well as to design X-ray window in x-ray operating tools which protects from several photons risk. The smaller TVL is, the superior the glass considered is, in shielding fields. There is an observable decreasing order in the TVL with the addition of  $TiO_2$  content. This emphasizes that LBZ-TV1 showed the best sample useful in shielding against gamma-rays. Fig. 6 shows that the minimum TVL is observed at 20 keV, while the highest TVL is observed at 1 MeV. The TVL also shows an increasing trend with increasing the energy. Similar outcomes were reported for different glasses [40–44].

For applying the studied glasses in real applications, especially those related to radiation shielding purposes, it is useful to compare the shielding properties of the studied glasses with some standard shields as well as with Pb-based and Pb-free glasses. In Fig. 7, we presented a comparison between the MFP of the LBZ-TVx glasses with those of different commercial shields. In Fig. 7, the ordinary and barite concretes were taken from Refs. [45], RS-360 and RS-253-G18 commercial glasses were taken from Refs. [46], Pb-free glass (AFZT5) was taken from Ref. [42], and Pb-based glass (TBZP10) was taken from Ref. [11]. This comparison was achieved over a wide photon energy range from 15 keV to 15 MeV that is very important in many radiation applications. Obviously, the MFP values of LBZ-TV1, LBZ-TV2, LBZ-TV3, LBZ-TV4, and LBZ-TV5 are lower than those of ordinary and barite concretes, and commercial glasses (RS-253-G18). This implies that the shielding properties of LBZ-TV1, LBZ-TV2, LBZ-TV3, LBZ-TV4, and LBZ-TV5 glasses are better than those of mentioned standard shields. Finally, the

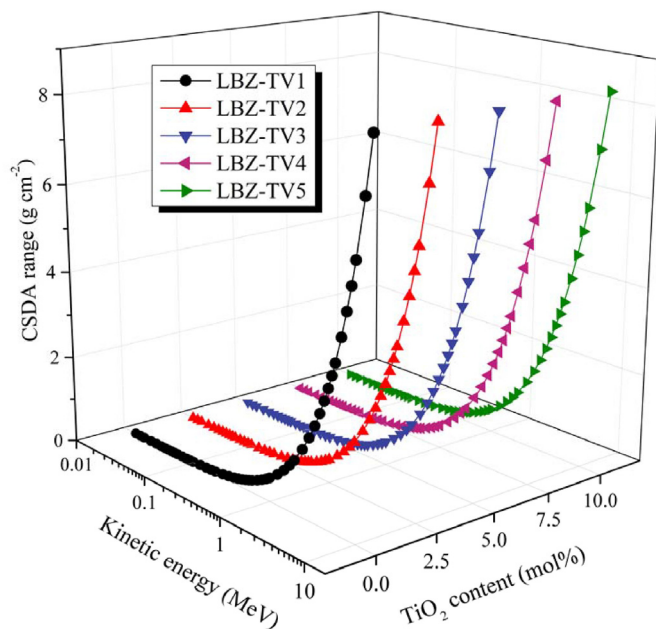


Fig. 9. Variation of the electron CSDA range ( $\Phi_e$ ) as a function of kinetic energy for LBZ-TVx glass system.

electron shielding properties were evaluated (as an example for the shielding against the charged particle) by determining the total stopping powers TSP ( $\Psi_e$ ) and CSDA range ( $\text{gm.cm}^{-2}$ ). The total stopping powers TSP ( $\Psi_e$ ) as a function of kinetic energy is shown in Fig. 8. It is clear that the  $\Psi_e$  values decreased as the kinetic energy of electron increased. The CSDA range ( $\text{gm.cm}^{-2}$ ) for each prepared sample is plotted against electron kinetic energy (MeV) and  $\text{TiO}_2$  content (mol%) as shown in Fig. 9. In all the tested glasses, the CSDAs increased as the kinetic energy of electron increased. Finally, it should mention that the effect of  $\text{TiO}_2/\text{V}_2\text{O}_5$  substitution was a little on the electron shielding properties of the tested glasses.

#### 4. Conclusion

In the present work, we used Geant4 Monte Carlo simulations to investigate the effect of  $\text{TiO}_2/\text{V}_2\text{O}_5$  substitution on the optical features and the properties of the radiation shielding for alkali borate glasses in the chemical form of  $30\text{Li}_2\text{O} + 55\text{B}_2\text{O}_3 + 5\text{ZnO} + x\text{TiO}_2 + (10 - x)\text{V}_2\text{O}_5$ , where  $x = 0, 2.5, 5, 7.5, \text{ and } 10$  mol%. The optical features such as  $R_m$ ,  $\alpha_m$ ,  $e^{\text{static}}$ ,  $e^{\text{optical}}$ ,  $T$ , and  $R_L$  were evaluated. The radiation shielding properties was estimated by determining TF, TVL, MFP,  $\Psi_e$  and  $\Phi_e$ . A good agreement was noticed between the results of Geant4 Monte Carlo and the theoretical calculations performed by XCOM platform. The results revealed that the  $\text{TiO}_2/\text{V}_2\text{O}_5$  substitution had a remarkable influence on the gamma shielding properties of the tested glasses. On the other hand, the optical properties slightly changed by the  $\text{TiO}_2/\text{V}_2\text{O}_5$  substitution. The properties of gamma shielding were compared with many samples in terms of MFP. The present glasses showed superior features to apply for optical and radiation shielding applications.

#### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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