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Impact of B₂O₃ on physical, optical characteristics and radiation attenuation factors of borotellurite glasses

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Abstract:

Borotellurite glasses with a composition [(60-X)TeO₂-(20+X)B₂O₃-10Li₂O-10Bi₂O₃] where x= 5-20 in steps of 5 mol% have been synthesized. Glass density, molar volume, oxygen packing density, and many other physical parameters were measured. UV-spectra in the wave length range (200-800) nm have been measured for the whole glass series. The optical energy band gap E_{opt} , refractive index, and optical basicity were measured. The mass absorption coefficients (μ_m) are determined experimentally by the HPGe detector and compared with the theoretical values obtained by XCOM program and MCNP5 simulation code within (0.121–1.408) MeV photon energy range. Half value layer (HVL), effective atomic number and electron density (Z_{eff} and N_{eff}), and macroscopic removal cross-section (ΣR) were evaluated. The sample [55TeO₂ – 25B₂O₃ – 10Bi₂O₃ – 10Li₂O] possess the highest values of ($\mu_m = 1.192 \pm 0.033$ cm²/g, $Z_{eff} = 56.12$ e/atom and $\Sigma R = 0.101499$ cm⁻¹) at energy 121 keV also lower values of (HVL = 0.121 cm, TVL = 0.1 cm and MFP = 0.174 cm) at photon energy 121 keV, therefore this sample considered the best gamma ray shielding material among the prepared glasses.

Keywords: Glasses; Optical properties; Radiation shielding; MCNP5 code; XCOM software.

1. Introduction:

Tellurite glasses have been created in binary, ternary, and quaternary forms since the early 1980s and have been examined as an excellent example of the new non-crystalline solids. For nearly four decades, research has focused on the development of new materials by modifying TeO₂ glass with rare earth (R.E.) or transition metal (TM) ions to obtain

interesting optical, electrical, thermal, and elastic properties; in addition, research articles about the structure of tellurite glasses have been published [1-10]

Today's the need for a shield to reduce harmful effects associated with a radiation dose is the only way, so the need to a transparent shield has become important especially in nuclear research laboratories, medicine (radio therapy), nuclear reactor (fission from 1 to 2 MeV) and agricultural in order to watch what happening inside the laboratory and monitor everything through it without the need to be exposed to harmful radiation that may cause serious damage that is difficult to repair. The most popular (concrete and lead); have some of disadvantages such as toxicity, opaque and poor product qualities. Glasses were examined among these materials by different researchers in the last several years with regard to purity and high absorption of radiation [11-15]. In general, (phosphorous, silicon, and boron) oxides are considered glass-formers. B_2O_3 - based glasses have gained popularity among the investigators and scientists because B_2O_3 - based glasses are relatively cheap, have good transparency and are compatible with the needed forms and dimensions. [16].

The principle purpose of this work to examine the optical and gamma protection characteristics of the present fabricated glasses $[(60-X)TeO_2 - (20+X)B_2O_3 - 10Li_2O - 10Bi_2O_3]$. The following items were carried out to achieve these goals:

- 1- TeO_2 - B_2O_3 - Li_2O - Bi_2O_3 glasses were prepared.
- 2- Many factors were measured in the structure of the synthesized glass.
- 3- UV measurements were carried out of the prepared glasses.
- 4- Many Optical features were estimated.
- 5- The mass absorption coefficient and many other related parameters were evaluated for the present fabricated glass samples experimentally and theoretically by using two programs (MCNP5 simulation code and XCOM).

2. Materials and method

2.1 Glass preparation

All glasses were prepared from pure chemicals (powder). Tellurium oxide TeO_2 , lithium oxide Li_2O as lithium carbonate Li_2CO_3 , boron oxide B_2O_3 , and bismuth oxide Bi_2O_3 were used in the this study. The amounts of the initial materials were weighted for each specimen depend on the equation $[(60-X)TeO_2 -$

(20+X)B₂O₃-10Li₂O-10Bi₂O₃] where x from (5-20) mol% by step 5, these glasses are up to (4.8248) g.cm⁻³ high in density. To produce homogenous blends, a mortar used for 10 minutes. The powder was heated in crucible of alumina at 500 °C for half hour in a muffle furnace. Then melted in a muffle oven for 20 min its temperature was raised gradually from (840 – 880) °C. For perfect homogeneity, crucibles have frequently been shaken. The transparent melt pressed with a steel rod and cooled at room temperature. At 300 °C each specimen annealed for 12 hours to reduce the crack. The glasses are polished to ensure that the surface is parallel, smooth and clear.

2.2 Physical properties

The density (ρ) of the studied glasses was calculated by using the law of Archimedes. Refined water was used as a dipping liquid. The 1st measurements were made in air (m_a), 2nd in water (m_w) of density $\rho_w = 1 \text{ g cm}^{-3}$. The density of the glass (ρ_g) calculated using the equation:

$$\rho_g = \left(\frac{m_a - m_w}{m_a} \right) \rho_w \quad (1)$$

The molar volume (V_m) of the present samples was deduced by:

$$V_m = \frac{M_{wt}}{\rho} \quad (2)$$

Where M_{wt} the molecular weight for all specimens were estimated from [5]:

$$M_{wt} = \sum m_k Z_k \quad (3)$$

Where m_k the ratio oxide component by mole.

Z_k each single oxide's molecular weight.

Oxygen packing density (OPD) is the arrangement of oxygen atoms of the glass system can be obtained as below,

$$OPD = 1000 \times C \times \frac{\rho_g}{M_{wt}} \quad (4)$$

Where C is the number of oxygens per formula unit.

Concentration of ions (N_i) (ions/cm³) of the fabricated glasses is given by Eq. (5) [17].

$$N_i = \frac{B_2O_3 \text{ mol\%} * \rho * N_A}{V_m} \quad (5)$$

Where N_A Avogadro's number.

Using the values of ion concentrations, Polaron radius (r_p) and Inter-nuclear distance (r_i) were calculated [17].

$$r_p = \frac{1}{2} \left(\frac{\pi}{6N} \right)^{1/3} \quad (6)$$

$$r_i = \left(\frac{1}{N} \right)^{1/3} \quad (7)$$

Which is the (r_i) the inter ionic distance between the two (B) ions.

The optical absorption spectrum of the finely shaped glass components about ~3 mm thickness were measured at room temperature using the double-beam spectrophotometer Perkin-Elmer 402 within wavelength range (200–800) nm.

2.3 Optical properties

In this work, the optical energy band gap (E_{opt}) was studied using two methods: Tauc's method and absorbance spectrum fitting (ASF) method). In the first method, Lambert – Beer – Bouguer law was used to calculate the optical energy band gaps for our glasses [18] via the absorption spectrum used.

$$\alpha(v) = \left(\frac{1}{t} \right) \ln \left(\frac{I_i}{I_t} \right) = \frac{2.303 A}{t} \quad (8)$$

Where $\alpha(v)$ the absorption of UV of the amorphous substance, (I_i) the incident intensity, (I_t) the transmitted intensity, (A) the absorbance of light and (t) is the thickness of each specimen. Eq. (8) has been generated by Tauc [18], then Mott and Davis [19] as:

$$\alpha h\nu = B(h\nu - E_{opt})^S \quad (9)$$

The incident gamma ray energy ($h\nu = E$), (B) is a constant and $S = 0.5$ and 2 for direct and indirect transition respectively. Plots of $(\alpha E)^2$ and $(\alpha E)^{1/2}$ versus (E) were drawn for all samples, values of (E_{opt})_{Tauc's} calculated, where $(\alpha E)^2$ and $(\alpha E)^{1/2} = 0$ [21].

In the (ASF) method, the optical band gaps directly mainly with the following equation by utilizing the absorption data, without the need for thickness of glass [21]:

$$E_{ASF} = \frac{hc}{\lambda_{(cut-off)}} = \frac{1239.83}{\lambda_{(cut-off)}} \quad (10)$$

Where the planck's constant, light velocity and (cut-off) wavelength are respectively, h , c , and $\lambda_{(cut.off)}$. Schemes of $\left(\frac{A}{\lambda} \right)^2$ and $\left(\frac{A}{\lambda} \right)^{1/2}$ with $\left(\frac{1}{\lambda} \right)$ were plotted for all glasses.

Urbach's energy (ΔE) for amorphous compound disarray evaluation; Urbach's lower energy values show a lower glass existence, estimated by the slope of plotting line $\ln(\alpha)$ against $(h\nu)$, in accordance with the empirical law of Urbach [21]:

$$\ln \alpha = \ln \alpha_0 + \left(\frac{h\nu}{\Delta E} \right) \quad (11)$$

The linear refractive index (n) was calculated for all samples using (E_{opt}) values [21]:

$$\frac{n^2 - 1}{n^2 + 1} = 1 - \sqrt{\frac{E_{opt}}{20}} \quad (12)$$

The molar refractivity (R_m), molar polarizability (α_m) and reflection loss (R_L) of the investigated glasses were estimated by [22]:

$$R_m = \left(\frac{n^2 - 1}{n^2 + 1} \right) \quad (13)$$

$$\alpha_m = \left(\frac{3}{4\pi N} \right) R_m \quad (14)$$

$$R_L = \left(\frac{R_m}{V_m} \right) \quad (15)$$

Depending on the metallization (M) values, the material kind (metallic or Insulator) [22]:

$$M = 1 - \left(\frac{R_m}{V_m} \right) \quad (16)$$

In addition, dielectric constants (static and optical) are estimated by the refractive index [22]:

$$\epsilon^{static} = n^2 \quad \text{and} \quad \epsilon^{optical} = n^2 - 1 \quad (17)$$

The electro-negativity (χ) of the studied glasses was determined by using (E_{opt}) as follow:

$$\chi = 0.2688 E_{opt} \quad (18)$$

Finally, the electro-polarizability (α°) and optical basicity (Λ) values have been computed by [22]:

$$\alpha^\circ = -0.9 \chi + 3.5 \quad (19)$$

$$\Lambda = -0.5 \chi + 1.7 \quad (20)$$

2.4 Gamma interaction with matter

As known photon can interact with matter via three processes photoelectric absorption (PE), Compton scattering (CS), and Pair production (PP). The total attenuation coefficient (μ_m) for photon from the three physical process ($\mu_{total} = \mu_{PE} + \mu_{CS} + \mu_{PP}$) [23]. The degree of attenuation depends on the dispersion and several absorption processes. The gamma ray detector has been used to measure the mass attenuation coefficient, utilize by HPGe detector. It has the following specifications: i) the efficiency of the detector is 24.5% for 1.333MeV, ii) the resolution is 2.2 keV at 1.333 MeV, iii) the detector surrounded by a thick lead shield about 10 cm, and is concentric with a Copper thin layer. (Genie 2000) Software is used to collect and analyze the gamma ray spectra. Both the gamma point source, and the Samples of glass have been housed and centered in a two collimators, lead shields with a very narrow hole in the center of the collimator, the upper cylinder (length 10 cm) its diameter = 0.5 cm which is equal to the diameter of the point source and the lower one (length 10 cm) its diameter = 1 cm. The source was at the top of the upper cylinder and it's covered with a lead cap, the glass samples placed at the end of the upper one in its cavity to ensure that it does not move during the measurements. All the lead system was placed inside the head of crystal by using a stand of wood. The reason to use two collimators to generate a narrow beam to minimized the systematical errors. ^{152}Eu point source with strength (290 ± 4) kBq emitting gamma ray photons with energies (0.121, 0.344, 0.778, 0.964, 1.112 and 1.408) MeV their emission abundance probabilities (28.37, 26.57, 12.97, 14.63, 13.54 and 20.85) % respectively which represented in Fig. 1a.

The intensity of gamma ray (I_0 and I) were measured by putting the glass specimen between the source and the crystal detector. The measured time was set to 3600 sec, the back ground radiation intensity was also measured for the same time and subtracted from each of the readings.

$$I = I_0 e^{-\mu_l x} \quad (21)$$

$$\mu_m = \ln(I_0/I) / \rho x \quad (22)$$

Where μ_m the mass absorption coefficient and x is the glass thickness (cm) which lies between (0.185 to 0.285) cm.

The mass absorption coefficient (μ_m) (cm^2/g) of the studied glasses was estimated theoretically by a mixture rule [11,12]:

$$(\mu_m)_{\text{glass}} = \sum_i w_i (\mu_m)_i \quad (23)$$

Where (w_i) and $(\mu_m)_i$ are weight fraction and mass absorption coefficient in the sequence of samples of the investigated element.

Also basic factors, half value layer (HVL) and tenth value layer (TVL) which define as, the thickness of the shield that reduces the initial intensity (I_0) by 50% and 10% respectively[11,12].

$$\text{HVL} = 0.693/\mu_l \quad (24)$$

$$\text{TVL} = 2.302/\mu_l \quad (25)$$

Where μ_l is the linear absorption coefficient ($I = I_0 e^{-\mu_l x}$)

The mean free path (MFP) of glasses which indicates to the average interval between two successive photon interactions can be calculated as [22]:

$$\text{MFP} = (\mu_l)^{-1} \quad (26)$$

The effective atomic number (Z_{eff}) and the effective ion density (N_{eff}) were estimated from [22]:

$$Z_{\text{eff}} = \frac{\sum_i f_i A_i (\mu_m)_i}{\sum_i \frac{A_i}{Z_i} (\mu_m)_i} \quad (27)$$

$$N_{\text{eff}} = \frac{N_A}{A_m} Z_{\text{eff}} \sum_i n_i \quad (28)$$

Where $\sum_i n_i$ total number of sample elements and A_m the glass atomic mass.

Using the mass removal cross section, the bioactive glass systems were assessed ($\Sigma R/\rho$) values of the elements in the shield material by using [22]:

$$\Sigma R = \Sigma W_i (\Sigma R/\rho)_i \quad (29)$$

Where W_i is the partial density ($W_i = w_i \rho_s$) where w_i is the fraction by weight of the i component and ρ_s is the sample density. To investigate the radiation shielding ability of prepared glass samples, the (μ_m) values have been estimated experimentally using HPGe detector as in Fig.1 a, theoretically by XCOM [24,25] and MCNP5 simulation code [25, 26] as in Fig. 1b.

3. Results and discussion

The density of the glass is usually considered an important parameter, because any change in the density of a glass indicates the change in the chemical composition and in the glass structure from Table 1. It can be shown that the density of a glass samples decreases while the molar volume is increases with the decrease in TeO_2 from (55 to 40) mol%

content also increase in the B_2O_3 from (25 to 40) mol% content. This is can be attributed to the replacement of higher atomic weight of TeO_2 (159.59 g/mol) by lighter atomic weight B_2O_3 (69.62 g/mol) content, so we can say there is a strong relation between the density and the glass structure [17]. From Table 1, the addition of B_2O_3 mol% content in the glasses decreases the compactness of the glass network. The large radius of B_2O_3 than TeO_2 increases the molar volume. The measured molar volume values showed an increasing trend, these mean that the molar volume and density are inversely proportion to each other as [28]. In the prepared glass specimens the decrease in the density is expected because the heavier oxide (TeO_2) was replaced by the lighter one (B_2O_3) which decrease the all molecular weight of the glass which is represented in Table 2. The molecular weight values ranged from (154.77 to 141.27) g/mol. The increase in molar volume as a result of the formation of NBO (non- bridging oxygen) which caused an opening structure by shattering the bonds, increasing in free volume, as shown in [27] the Tellurium oxide replaced by Boron oxide. The OPD (oxygen packing density) increased from (70.14 to 73.78) mol/L by raising the boron oxide content from (25 to 40) mol% content because of increased the oxygen atom number per unit composition from (2.25 to 2.4) oxygen atom fraction. This behavior is attributed to the fraction of oxygen atom when tellurium oxide replaced by boron oxide is equal (3: 2) respectively which agreement with research [28]. Other physical parameters such as the ion concentration B_{ions} (N_i) are increased with increase the concentration of B_2O_3 values according to Table 2, polaron radius (r_p) and inter- nuclear distance (r_i) are estimated by using Eqs. (5-7). It shown that the values of r_p and r_i varies with the addition of boron oxide content in the glasses. The value of r_p decrease with the increase of B_2O_3 mol% into glass, which mean that the average space of B-B or r_i shows decrease trend, the r_p of each glass specimen smaller than the B-B spacing there is a good agreement with the polaron theory, that the r_i must be greater than the r_p on which the electron localized as seen in the study estimated by [29].

With increased B_2O_3 mol% the absorption edge shifts to higher wavelengths Fig.3. The E_{opt} is the change of energy among conduction and valence bands of the glass when the energy of an incident light greater than the energy band gap the transition will occur [28]. The optical energy band gap calculated by Tauc's method by Eq. (9) for direct (E_{opt})_{Tauc's} of glasses as shown in Fig. 4a, which varied between (2.8975 to 2.7312) eV deduced in Table 3. Fig.

4b represents the values of indirect $(E_{opt})_{Tauc's}$ of the glass samples changed between (2.6842 to 2.4571) eV when boron content increase. There is a decrease in E_{opt} with rising in boron content which it's attributed to the formation of (NBO) as discussed before, also an increase of the disorder and increase in the nature of amorphous of the glass samples. The energy needed to excited the electron in the case of the (NBO) is smaller than the (bridging oxygen), which facilitates to shift the valence band to the conduction band which in turn decreases the optical energy band gap as studied [28]. Calculations of E_{opt} from Eq. (10) which represented in Figs. (5a and 5b), showed that the direct $(E_{opt})_{ASF}$ of the glass samples have high values (2.8875) eV, but have value (2.7234) eV for indirect transition as the B_2O_3 mol% content increases. The observations of (E_{opt}) values realized by two techniques have been confirmed at Table 3.

By using Eq. (12), the calculated values of the refractive index which represented at Table 3. The values of (n) estimated by two methods for direct and indirect transitions increasing with the increase of boron oxide mol% content. This is due to the high polarity of the third boron ion (B^{3+}) which break (bridging oxygen (BO)) to form (non- bridging oxygen (NBO)) which have high polarity, so (NBO) affected on the value of the refractive index. These synthesized glass samples are characterized by its high refractive index by compare with glasses studied by [15, 29]. An Urbach energy: the measure of disorder of the glasses and calculated by Eq. (11). This represented at Table 2. The increasing in the B_2O_3 from (25 to 40) mol% content, the values of Urbach energy increased from (0.263 - 0.327) eV which it means that the disorder of boron samples increased, with increased the defect in the glass samples and forming the (NBO) [28, 29].

The R_m values increases from 26.624 to 27.209 ($cm^3.mol^{-1}$) with increasing of B_2O_3 mol% as shown in Table 2. The R_m is correlated to the molar polarizability of a material (α_m) as deduced by Eq. (14). The resultant values of (α_m) increase from 10.559×10^{-24} to 10.792×10^{-24} ($cm^3.mol^{-1}$) with increasing B_2O_3 mol% as tabulated in Table 2. Accordingly, increasing the R_m is in direct relation with increases the glass polarizability which agreement with research [30].

Metallization of the glass specimen is used to know the nature of the solid based on the values of refractive index to deduce the nature of the solid and depend on the reflection loss

(R_L) with using Eq. (16). The rule of thumb being used is (R_m / V_m) < 1 (is non-metallic) and if (R_m / V_m) > 1 (is a metallic). In this study the decrease of calculated values of metallization ranged from (0.170 - 0.163) which indicates that the type of the synthesis glass is non-metallic which represented in Table 2.

The dielectric constants (ϵ^{static} , $\epsilon^{\text{optical}}$) calculated by Eq. (17) are exactly proportionate to each other but reverse with a metallization characteristic (M) that is good agreement with work [22].

The electro-polarizability is a parameter used to specified the nature of the bonds present in the solid and calculate it. As summarized in Table 2. When the boron oxide mol% increase the polarizability of increased from (2.799 to 2.839) this can be due to the breaking of Te-O-Te bond when B ions is injected into the network and produce a non-bridging oxygen. So that NBO possess high polarizability values. The values of electro-negativity (χ) which calculated by Eq. (18) based on (E_{opt}) see Table 2. The electro polarizability (α°) displayed at Fig. 9, optical basicity (Λ) at Fig. 10 were calculated by Eqs. (19 and 20) respectively. With increasing the B_2O_3 mol%, (α°) and (Λ) values are increased. The strongly polarizable of B_2O_3 relative to TeO_2 leads to enhanced in optical basicity (Λ).

Optical basicity values ranged from (1.311 to 1.333) see Table 2. With the boron oxide content increase, this shows that the polarizability of the glass samples increases as shown for refractive index. This increase in polarizability showed that there is an increase in NBO content.

The experimental results of the mass attenuation coefficient μ_m showed in Table 4 for boron concentrations ranged from (25 to 40) mol% contents calculated experimentally by HPGe detector with the aid of Eq. (22) which compare with values estimated theoretically using MCNP5 simulation code and XCOM programs throughout (0.121, 0.343, 0.778, 0.964, 1.112 and 1.408) MeV photon energy. Perfect agreement within μ_m obtained from the experimental data and the values obtained from MCNP5 code. According to this performance, Fig. 11, which represent the behavior of mass attenuation coefficient obtained by the three methods and compare between them for all concentration of B_2O_3 , significant declines in (μ_m) with increasing the photon energy from (0.121 to 1.408) MeV. The values obtained from XCOM program differ from the EXP and MCNP5 code, this may be attributed to the weakness of the XCOM program, which it doesn't take into account the

shape, thickness of the sample, type of the detector also the geometry of the system, so these are a clear defects in that program. Fig. 12 shows that the mass attenuation coefficient of different boron mol% content and their variations with gamma ray energies. It is clear that all the samples have nearly the same behavior; it is obvious that the μ_m values of all glass samples dramatically decrease with the increase of photon energy from (121 to 343) keV (photoelectric process (PE)) is the dominant mechanism at low energy as (σ_{PE}) proportion with $E^{-7/2}$. Then slightly decrease of (μ_m) with the increasing of the photon energy. But From (778 to 964) keV there is no significant decrease in μ_m values with gamma energy and the values are approximately constant for all samples due to Compton scattering (CS) the more influenced interaction, cross -section (σ_{CS}) is proportional to the energy of photons E^{-1} . Up to ~ 1020 keV the mass attenuation slightly increase but still approximately constant for all glasses, this behavior of the attenuation with gamma energy may be attributed to pair production (PP), μ_m values are decrease with increasing energy due to cross section (σ_{pp}) directly proportion with energy E in the third region from (1112 to 1408) keV slightly with the effect from Compton Scattering which decreases.

From the above results it have been concluded that the higher probability of photon interaction with glass samples occurs in the lower photon energy. From Table 4 the gamma radiation attenuation don't change with addition of B_2O_3 mol% content in the synthesized glasses from (25 to 40) mol% content. Thus the power of the complex materials can be concluded as follow: Bi (heavy element) is the main element for shielding gamma ray using in this work have a small influence on the shielding properties against gamma ray because its content in all samples is constant (Bi = 10 mol%), but boron which varying in these glasses not sufficient to affected on the gamma shielding, therefore there is no change in μ_m values, the reason to use B in our prepared glasses, B act as a glass former. We can note that it can be used as a good neutron shield (light element). Finally the perfect boron sample in gamma shielding is the sample (55 TeO_2 , 25 B_2O_3 , 10 Bi_2O_3 and 10 Li_2O) mol% content which possess the high density (4.8248) g/cm^3

The variance in the experimental values of HVL of our prepared glasses ($TeO_2 - B_2O_3 - Bi_2O_3 - Li_2O$) with different percentage (mol%) have been calculated by Eq. (24) with the help of μ_m values Fig. 13 shows that the minimum values for HVL was found at photons with low energy this attributed to the main affected interaction is photoelectric effect (PE) dominance (due to there is no effect from low Z of Boron

according to ($\sigma_{PE} \propto \frac{Z^5}{E^{7/2}}$)). Increased gradually with the increase of photon energy (> 0.5 to 0.964) MeV the PE probability decrease and Compton scattering probability increased where ($\sigma_{CS} \propto \frac{1}{E}$). At energy Zone up to 1.02 MeV there is a significant increase in HVL values due to the dominant interaction in this zone is pair production where ($\sigma_{PP} \propto E$) which mean that pair production interaction its probability increase with photon energy. For all samples selected, a fast increase in HVL with photon energy, have maximum value at 1.408 MeV for all samples attributed to the ($\sigma_{PP} > \sigma_{CS}$) and Compton scattering decrease; Also from Fig. 13, the sample (B 25 and Te 55) mol% content possess the lower HVL (0.121 cm) at energy 121 keV and (2.9 cm) at energy 1408 keV, its lower values represented that shield is more effective between our prepared glasses. The HVL for B25 is less than all the glasses tested by [31, 32].

The TVL and MFP have the same behavior as HVL, these values calculated by using Eqs. 25 and 26 with the variation of B₂O₃ from (25 to 40) mol% content at the selection energy as shown in Figs. 14 and 15. The experimental values of these parameters are various with photon energy from (121 to 1408) keV, from TVL and MFP figures, it is obvious from these curves there are a dramatically increase with photon energy, at energy zone from (121 to 343) keV these parameters have the smallest values due to the main interaction affected in this is (photoelectric process), which its probability inversely proportion with energy by $E^{-3.5}$. With increasing the photon energy the values of these parameters increases which attributed to the (Compton scattering) is dominant interaction. At energy up to 1.02 MeV there is a rapid increase in these values with energy for all glasses due to the pair production is dominant interaction. Also, Figs. 14 and 15 showed that sample (25 B₂O₃ and 55 TeO₂) mol% content possess the lower TVL (0.4 and 9.64) cm at energies (121 and 1408) keV respectively, for MFP (0.174 and 4.19) cm at energies (121 and 1408) keV respectively. The reduction in these parameters with energy is the good ability of these shields to attenuate primary radiation.

The Z_{eff} values of the investigated samples are estimated by using Eq. (27), the variation of Z_{eff} for the prepared glasses with energy is displayed in Fig. 16, which represented the effective atomic number Z_{eff} of all glasses with photon energy. The values of Z_{eff} of the fabricated glasses decreases with the replacement of (TeO₂ by B₂O₃) see Fig. 16, the values of Z_{eff} is 56.12 (e/atom) at 121 keV and

19.24 (e /atom) at energy 1408 keV for glass sample (B25) as seen in Table 1, which displayed the values of Z_{eff} is 54.87 (e/atom) at 121 keV and 16.5 (e/atom) at energy 1408 keV for glass sample (B40). A rapid decrease in the value of Z_{eff} after 0.1 MeV, because the photoelectric dependent on photon energy as $E^{-7/2}$, but Z_{eff} values are mainly constant up to 0.9 MeV where the controlling interaction at this energy zone is Compton scattering, while for energy ($1.02 \text{ MeV} < E < 1.2 \text{ MeV}$) Z_{eff} values increases with gamma energy which due to dominant of (pair production) and the (Compton effect), then after that remarkable decreasing for Z_{eff} curve can be showed with photon energy, the (Compton scattering) plays a neglected role. From Fig. 16 B25 is the best form of synthesized glasses in this high energy area for gamma shielding. This result also shows that a composition of glass has an important function in gamma protection.

The effective ion density calculated from the experimental results by using Eq. (28) for (B25, B30, B35 and B40) with the photon energy in the region (121 to 1408) keV, represented in Fig. 17. One may observe that N_{eff} have the opposite relation with atomic mass (A_m) ($N_{\text{eff}} \propto \frac{1}{A_m}$). Where A_m for the glass samples varies from (41.53 for sample B20 to 35.32 for sample B40), so as we see the value of A_m decrease with increasing the boron content, therefore values of N_{eff} increase with boron content change from (25 to 40) mol%.

The variation of μ_m versus B_2O_3 mol% content at energies from (121 to 1408) keV deduced in Fig. 18. The figure indicates that the B content not influenced on the values of μ_m at higher energies greater than (0.343 MeV), but on the other hand the μ_m from experimental results have high values at low energy zone at (121 and 343) keV the main reason for that behavior can explained as follow:

- 1) At $E = 121 \text{ keV}$, the photoelectric absorption effect is the dominant interaction ($\sigma_{\text{PE}} \propto E^{-7/2}$).
- 2) At $E = 343 \text{ keV}$, the effect of photoelectric is weak effect so that μ_m have a slightly high values.
- 3) Up to 600 keV, there is no effect from PE but CS is the dominant interaction in the two lines (778 and 964) keV, therefore there is a decrease in μ_m for all glasses.

4) Up to 1020 keV, at $E = 1112$ keV and 1408 keV, the effect of PP is clear and dominant and approximately constant also there is no effect for B content in these energies due to the small values of M_{wt} .

The macroscopic effective removal cross section (ΣR):

Using Eq. (29), the results are shown in Fig. 19 and listed in Table 5. It can be viewed from the figure that ΣR of the glass samples are quite near to each other and ranged from (0.101499 to 0.100936) cm^{-1} for samples ranged from (B25 to B40) mol% content. The relatively high effective removal cross-section of sample (B25) seen in Table 5. Can be explained by its higher density (4.8248 g/cm^3) than the other samples (see Table 1), also can be seen that the sample (B40) which already has lower density (4.3433 g/cm^3) has lower ΣR value, therefore the results presented in Table 5 indicate that the density of the glass is an important parameter in neutron attenuation. As a result, it can be said that the sample (25 B_2O_3 , 55 TeO_2 , 10 Li_2O and 10 Bi_2O_3) is the most appropriate sample among all prepared glasses.

It was observed that the values of ΣR values of the present tellurite glasses were greater than [34, 35]. In the future studies, we will take the Boron with low (mol%) content ranging (15 to 30) and compare between them to find the best shield for neutrons.

4. Conclusion

Glass compositions [(60-X) TeO_2 - (20+X) B_2O_3 -10 Li_2O -10 Bi_2O_3], showed that:

- Density decreases from (4.8248 to 4.3433) g/cm^3 by increasing the B_2O_3 due to the replacement of higher atomic weight of TeO_2 (159.59 g/mol) by lighter atomic weight B_2O_3 (69.62 g/mol).
- E_{opt} reduces when B_2O_3 mol% content rises due to the structural configuration which is attributed to the formation of (NBO).
- Optical basicity values ranged from (1.311 to 1.333) With the boron oxide content increase, this shows that the polarizability of the glass samples. This increase in polarizability showed that there is an increase in NBO content.
- The maximum (μ_m) values observed for sample B25 investigated that to become a good absorber material against gamma radiation. With low photon energy (< 500 keV) the best attenuation for gamma occurs.

- The value of Z_{eff} of the prepared glasses decreases with the replacement of TeO_2 by B_2O_3 . Up to 1020 keV it is a fast increase for Z_{eff} values due to (σ_{CS} , σ_{PP}) are dominant, at 1150 keV due to CS is neglected and the PP process is the most affected interaction the Z_{eff} decrease.
- The relatively high effective removal cross-section of sample (B25) is 0.101499 cm^{-1} can explained by its higher density (4.8248 g/cm^3) than the other samples.

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Table 1: Sample code, composition, density, molar volume, oxygen packing density and the photograph of the [(60-X) TeO₂-(20+X) B₂O₃ -10 Li₂O - 10 Bi₂O₃] glasses where X = 5, 10, 15 and 20 mol%.

Sample code	Composition (mol%)				ρ (g / cm ³)	V_m (cm ³ /mol)	OPD $\pm$ 0.1 (mol/liter)	Photograph of synthesized glass samples
	TeO ₂	B ₂ O ₃	Bi ₂ O ₃	Li ₂ O				
B25	55	25	10	10	4.8248	32.0776	70.1423
B30	50	30	10	10	4.6643	32.2169	71.3910
B35	45	35	10	10	4.5038	32.3661	72.6068
B40	40	40	10	10	4.3433	32.5263	73.7864

Table 2: Various physical and optical parameters of the prepared glasses.

<i>Sample Code</i>	<i>Optical energy band gab, E_{opt} (eV)</i>				<i>Linear refractive index, n</i>			
	<i>(E_{opt}) Tauc's</i>		<i>(E_{opt})_{ASF}</i>		<i>Tauc's method</i>		<i>ASF mothod</i>	
	<i>Direct</i>	<i>Indirect</i>	<i>Direct</i>	<i>Indirect</i>	<i>Direct</i>	<i>Indirect</i>	<i>Direct</i>	<i>Indirect</i>
B25	2.8975	2.6842	2.8875	2.7234	2.4252	2.4877	2.4280	2.4758
B30	2.8050	2.5443	2.8151	2.5763	2.4516	2.5319	2.4487	2.5216
B35	2.7897	2.5094	2.7787	2.5503	2.4561	2.5435	2.4594	2.5300
B40	2.7312	2.4571	2.7189	2.4747	2.4735	2.5610	2.4802	2.5551

Table 3: Optical energy band gaps and refractive indices of synthesized glasses obtained by Tauc's and ASF methods.

<i>Parameter</i>	B25	B30	B35	B40
<i>Number of oxygen atom</i>	2.25	2.3	2.35	2.4
<i>Molecular weight M_{wt} (mol)</i>	154.77	150.27	145.77	141.27
<i>Ion concentration (N_i) $\ast 10^{20}$ (ions/cm³)</i>	26.287	37.390	55.827	74.069
<i>Polaron radius r_p (Å)</i>	2.919	2.596	2.271	2.067
<i>Inter-nuclear distance r_i (Å)</i>	7.245	6.443	5.637	5.130
<i>Molar Refractivity R_m (cm³/mol)</i>	26.624	26.857	27.002	27.209
<i>Molar Polarizability ($\alpha_m \ast 10^{-24}$ cm³)</i>	10.559	10.652	10.709	10.792
<i>Metallization (M)</i>	0.170	0.166	0.165	0.163
<i>Reflection loss (R_L)</i>	0.173	0.176	0.177	0.179
<i>Electro-negativity (χ)</i>	0.778	0.754	0.749	0.734
<i>Electro-Polarizability (α°)</i>	2.799	2.821	2.825	2.839
<i>Optical basicity (Λ)</i>	1.311	1.323	1.325	1.333
<i>Urbach energy (ΔE) (eV)</i>	0.263	0.275	0.303	0.327
<i>Static dielectric constant, ϵ^{static}</i>	5.882	6.011	6.033	6.118
<i>Optical dielectric constant, $\epsilon^{optical}$</i>	4.882	5.011	5.032	5.118
<i>Optical transmission, T</i>	0.705	0.699	0.698	0.695

Table 4: Shows the mass attenuation coefficient (μ_m) values obtained experimentally (EXP) and theoretically by MCNP5 simulation code and XCOM program for samples (B 25, B 30, B 35 and B 40) at different photon energy.

Photon energy	B25			B30		
E (MeV)	EXP	MCNP5	XCOM	EXP	MCNP5	XCOM
0.121	1.192±0.033	1.083	1.422	0.955±0.035	0.937	1.423
0.343	0.181±0.008	0.139	0.166	0.133±0.008	0.137	0.166
0.778	0.073±0.016	0.063	0.073	0.071±0.018	0.061	0.073
0.964	0.063±0.015	0.054	0.063	0.062±0.012	0.054	0.063
1.111	0.057±0.020	0.051	0.057	0.052±0.017	0.051	0.057
1.408	0.050±0.009	0.042	0.050	0.043±0.009	0.042	0.050
Photon energy	B35			B40		
E (MeV)	EXP	MCNP5	XCOM	EXP	MCNP5	XCOM
0.121	1.051±0.031	1.023	1.424	1.008±0.039	1.005	1.424
0.343	0.170±0.008	0.139	0.167	0.155±0.008	0.139	0.168
0.778	0.073±0.020	0.062	0.073	0.073±0.016	0.063	0.073
0.964	0.063±0.015	0.054	0.063	0.063±0.014	0.055	0.063
1.111	0.057±0.016	0.052	0.058	0.054±0.017	0.052	0.058
1.408	0.050±0.009	0.042	0.050	0.050±0.009	0.042	0.050

Table 5: The macroscopic fast neutron removal cross –section of the prepared glass system.

Element	B25 $\rho = 4.8248 \text{ g/cm}^3$			
	$\Sigma_R \text{ (cm}^{-1}\text{)}$	fraction by weight	partial density (g/cm ³)	$\Sigma_R \text{ (cm}^{-1}\text{)}$
Te	0.029317	0.453452	2.187815	0.029317
O	0.045450	0.2325971	1.122234	0.045450
B	0.009689	0.0349264	0.168513	0.009689
Bi	0.013408	0.2700558	1.302965	0.013408
Li	0.003635	0.0089695	0.043276	0.003635
Element				0.101499
	B30 $\rho = 4.6643 \text{ g/cm}^3$			
	$\Sigma_{R/\rho} \text{ (cm}^2\text{/g)}$	fraction by weight	partial density (g/cm ³)	$\Sigma_R \text{ (cm}^{-1}\text{)}$
Te	0.0134	0.4245708	1.980326	0.026536
O	0.0405	0.2448843	1.142214	0.046260
B	0.0575	0.0431665	0.201342	0.011577
Bi	0.0103	0.2781409	1.297333	0.013350
Li	0.0840	0.0092381	0.043089	0.003619
Element				0.101342
	B35 $\rho = 4.5038 \text{ g/cm}^3$			
	$\Sigma_{R/\rho} \text{ (cm}^2\text{/g)}$	fraction by weight	partial density (g/cm ³)	$\Sigma_R \text{ (cm}^{-1}\text{)}$
Te	0.0134	0.3939068	1.774077	0.023773
O	0.0405	0.2579301	1.161666	0.047047
B	0.0575	0.0519152	0.233816	0.013444
Bi	0.0103	0.2867252	1.291353	0.013288
Li	0.0840	0.0095232	0.042891	0.003603
Element				0.101155
	B40 $\rho = 4.3433 \text{ g/cm}^3$			
	$\Sigma_{R/\rho} \text{ (cm}^2\text{/g)}$	fraction by weight	partial density (g/cm ³)	$\Sigma_R \text{ (cm}^{-1}\text{)}$
Te	0.0134	0.3612899	1.569190	0.021027
O	0.0405	0.2718067	1.180538	0.047812
B	0.0575	0.0612211	0.265902	0.015289
Bi	0.0103	0.2958563	1.284993	0.013223
Li	0.0840	0.0098264	0.042679	0.003585
				0.100936

Fig.1a: Schematic experimental setup arrangement. The diagram shows the lead collimators, the sample position and co- axial HPGe detector.

Fig.1b: MCNP5 simulation setup obtained from MCNP5 visual editor for mass attenuation coefficient.

Fig.2: The variation of density and molar volume vs. B_2O_3 mol% for all studied glass samples

Fig. 3: Optical absorption spectra of the glass samples.

Fig. 4a: Variation of $(\alpha h\nu)^2$ vs. $(h\nu)$ for glass samples (direct)_{Tauc's} method.

Fig. 4 b: Variation of $(\alpha h\nu)^{0.5}$ vs. $(h\nu)$ for glass samples (indirect)_{Tauc's} method.

Fig. 5a: Variation of $(A/\lambda)^2$ vs. $(1/\lambda)$ for glass samples (direct)_{ASF} method.

Fig. 5b: Variation of $(A/\lambda)^{1/2}$ vs. $(1/\lambda)$ for glass samples (indirect)_{ASF} method.

Fig.6: the graph represents the variation of $\ln\alpha$ vs. $h\nu$ (eV) for all glass samples.

Fig. 7: Variation of R_m and α_m with B_2O_3 mol% for all glasses.

Fig. 8: Variation of M and ϵ^{static} with B_2O_3 mol% for all glasses.

Fig. 9: Variation of α° and χ vs. B_2O_3 mol% for all glasses.

Fig. 10: Variation of α° and Λ with B_2O_3 mol% for all glasses.

Fig.11: Variation of mass attenuation coefficient (cm^2/g) of glass samples based on B_2O_3 mol% content with photon energy calculated by experimental method and theoretically by XCOM and MCNP5 simulation code.

Fig.12: Mass attenuation coefficient (μ_m)_{EXP} of the glasses as a function of the photon energy

Fig. 13: Half value layer (HVL) of the all glasses as a function of the photon energy.

Fig. 14: Tenth value layer (TVL) of the glasses as a function of photon energy.

Fig. 15: Mean free path (MFP) of the glasses as a function of photon energy.

Fig. 16: Effective atomic number (Z_{eff}) of the glasses as a function of photon energy.

Fig. 17: Variation of effective ion density (N_{eff}) values of all glasses at different photon energies.

Fig. 18: Dependence of μ_m (cm^2/g) values on the B_2O_3 mol% content.

Fig.19: Fast neutron removal cross sections Σ_R values for fabricated glass samples.