



## Journal of Advanced Research in Fluid Mechanics and Thermal Sciences

Journal homepage:  
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ISSN: 2289-7879



# Simulation-Based Radiation Shielding and Optical Properties of Thulium-Doped Bismuth Tellurite Glass

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### ARTICLE INFO

### ABSTRACT

#### Article history:

Received 18 August 2024

Received in revised form 12 November 2024

Accepted 24 November 2024

Available online 10 December 2024

#### Keywords:

Thulium doped bismuth tellurite; structural properties; radiation shielding properties; optical properties; lead-free glass

Lead-based radiation shielding material is currently used in industry to shield against high-penetration radiation such as gamma rays. However, lead is harmful to humans, animals, and plants. This study proposed a new composition of transparent lead-free glass. Using the melt and quench technique, thulium-doped bismuth tellurite glass with composition  $(\text{TeO}_2)_{1-x}(\text{Bi}_2\text{O}_3)_x(\text{Tm}_2\text{O}_3)_{0.02}$  where  $x = 0.05, 0.10, 0.15,$  and  $0.20$  mol % was fabricated. Significantly, the glasses with  $\text{Bi}_2\text{O}_3$  concentration of 5 mol % and 10 mol% have a higher density than the commercial glass containing lead indicating the fabricated glasses would perform better as a radiation shielding material. Comparing the simulated-radiation shielding properties using software Phy-X and XCom, the glass with 10 mol% of  $\text{Bi}_2\text{O}_3$  performs better as radiation shielding material than 5 mol% of  $\text{Bi}_2\text{O}_3$ . Meanwhile, glass with 5 mol% of  $\text{Bi}_2\text{O}_3$  performs better than 10 mol% of  $\text{Bi}_2\text{O}_3$  in terms of optical properties. Considering both radiation shielding and optical properties, the fabricated lead-free glass can be widely used in radiation shielding applications that require transparency.

## 1. Introduction

Currently, transparent radiation shielding glass is used in the medical industry as viewing windows to protect healthcare personnel during radiation treatment. However, like a double-edged sword, current radiation shielding glass used in industry contains lead which poses hazardous effects on humans, animals, and plants [1-5]. With the toxicity of lead, alternative development of lead-free radiation shielding glass became crucial. Despite numerous research efforts to develop lead-free glass, it is not easy to compose a glass composition that has high density and clear transparency that

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<https://doi.org/10.37934/arfmts.125.1.112126>

is at par with lead glass [6-9]. Therefore, a new composition of lead-free radiation shielding glass was proposed.

The chemical compounds of tellurium dioxide ( $\text{TeO}_2$ ), bismuth trioxide ( $\text{Bi}_2\text{O}_3$ ), and thulium (III) oxide ( $\text{Tm}_2\text{O}_3$ ) were incorporated into the glass composition. Tellurite-based glass is chosen as the glass base mainly due to its high density.  $\text{TeO}_2$  has a higher density of  $5.67 \text{ g/cm}^3$  compared to commercially used silicon dioxide ( $\text{SiO}_2$ ) with a density of  $2.65 \text{ g/cm}^3$ . This high density indicates that there is a high potential to be applied as a radiation shielding material since there will be a higher probability of interaction between atoms and harmful radiation such as gamma rays. The interaction of atoms could be either photoelectric effects, pair-productions, or Compton scatterings [10]. Previous studies have shown that glasses with a high density resulted in a high mass attenuation coefficient [11,12]. The mass attenuation coefficient expresses how many photons a homogeneous absorber removes per unit mass from a radiation beam such as x-rays or gamma rays. Apart from that,  $\text{TeO}_2$  glasses have a low melting temperature making them a good eco-friendly alternative due to their low energy consumption during the melting process [13]. Also,  $\text{TeO}_2$  glasses are transparent in the near UV to mid-IR wavelength range making it suitable to be applied in application that requires the line-of-sight [14]. Then,  $\text{Bi}_2\text{O}_3$  was incorporated into the glass composition due to its high density and non-toxic to the environment. In wastewater treatment, bismuth nanoparticles have been used to degrade dye, and a toxicology study proved that the treated dye water is non-toxic [15]. In terms of radiation shielding, when bismuth was layered together with a leaded gonad shield, bismuth significantly reduced radiation dose without disrupting the image quality of pelvic X-ray [16]. Hence, this shows the potential of bismuth as a radiation-shielding material. Furthermore,  $\text{Tm}_2\text{O}_3$  incorporation was found to improve glass structure by improving the connectivity of the glass network and atomic arrangement cross-linkage [17,18]. It was proven that  $\text{Tm}_2\text{O}_3$  incorporation in the  $\text{TeO}_2$  glass system significantly increases the mass attenuation coefficient and linear attenuation coefficient [19,20].

Taking into account the aforementioned considerations, a series of new compositions of tellurite-based glass was fabricated and the optical as well as radiation shielding properties were investigated. The radiation shielding investigation for the mass attenuation coefficient was conducted at a continuous energy range of 0.001 keV to 1000 MeV. Then, further analysis of radiation shielding at energy 0.662 MeV using Cs-137 was conducted. This energy was specifically chosen since the gamma rays with wavelength 0.001874 nm are usually applied in medical procedures such as radiotherapy [21]. Also, a comparison between fabricated glasses with industrial lead glass was made. This study can significantly contribute to the development of lead-free glass that is not only eco-friendly but also can be widely used in transparent radiation shielding applications in the medical industry.

## **2. Methodology**

### *2.1 Glass Samples Fabrication*

New composition of  $(\text{TeO}_2)_{1-x} (\text{Bi}_2\text{O}_3)_x (\text{Tm}_2\text{O}_3)_{0.02}$  where  $x = 0.05, 0.10, 0.15, 0.20$  mol % was fabricated using melt and quench technique. This fabrication technique was chosen due to its simplicity. After stoichiometry calculation, the chemicals of  $\text{TeO}_2$ ,  $\text{Bi}_2\text{O}_3$  and  $\text{Tm}_2\text{O}_3$  supplied from Alfa Aesar with 99.99% purity were weighted using a PGW 214 analytical balance from AE Adam. The weighted chemical was then transferred to a natural agate mortar and pestle. To ensure the chemicals were mixed homogeneously, the chemicals were grounded for an hour. After grounding, the chemicals were then transferred to an alumina crucible for the preheating process in an electric furnace. After an hour of preheating at  $400 \text{ }^\circ\text{C}$  to eliminate water vapour, the melting process was carried out in a different furnace for an hour at  $900 \text{ }^\circ\text{C}$ . While the melting process occurred, a

stainless-steel mould was heated at 400 °C to avoid thermal shock on the high-temperature molten sample. This thermal shock could cause the glass sample to have a higher susceptibility to crack during the annealing process. Following the melting process, the molten sample was poured onto a heated stainless-steel mould and placed in an electric furnace to undergo an additional 1 hour of annealing at 400 °C. The sample was then allowed to cool to ambient temperature.

## 2.2 Density and Molar Volume Measurement

The density measurement was conducted using an MGS-300 density meter from Alfa Mirage. Archimedes's principle was applied, and Eq. (1) was used for the calculation of the glass density.

$$\rho_{glass} = \left( \frac{w_{air}}{w_{air} - w_{water}} \right) (\rho_{water}) \quad (1)$$

where the symbol  $\rho_{glass}$ ,  $\rho_{water}$ ,  $w_{air}$  and  $w_{water}$  referred to glass density, water density, glass weight in air and glass weight in distilled water, respectively.

The molar volume ( $V_m$ ) of fabricated glass was calculated using the Eq. (2).

$$V_m = \left( \frac{M_m}{\rho_{glass}} \right) \quad (2)$$

The symbol  $M_m$  in Eq. (2) stands for the relative molar mass of glass samples.

Using the value of  $V_m$ , oxygen packing density ( $OPD$ ) was calculated using Eq. (3) [22].

$$OPD = \frac{1000 \times c}{V_m} \quad (3)$$

where  $c$  represent the number of oxygens per unit formula.

## 2.3 Structural Properties Characterization

Structural characterization was conducted by Fourier Transform Infrared Spectroscopy (FTIR). The FTIR measurement was conducted from 600  $\text{cm}^{-1}$  to 4000  $\text{cm}^{-1}$  wavenumbers using a Perkin Elmer FT-IR Spectrometer Frontier. FTIR measurement enables the analysis of the network in the glass structure. The examined glasses were in the form of solid glass samples.

## 2.4 Theoretical Radiation Shielding Properties Measurements

Web-based radiation shielding software Phy-X and XCom were used to measure the radiation shielding parameters such as mass attenuation coefficient ( $MAC$ ), half-value layer ( $HVL$ ), and mean free path ( $MFP$ ) of glass samples. For software Phy-X, the radiation shielding parameters were obtained directly from the software. However, for software XCom, radiation shielding parameters such as  $HVL$  and  $MFP$  were obtained through manual calculation since only  $MAC$  value can be obtained directly from the software. Using the value of linear attenuation coefficient ( $LAC$ ) as shown in Eq. (4), the value of  $HVL$  and  $MFP$  were calculated using Eq. (5) and Eq. (6), respectively.

$$LAC = MAC \cdot \rho_{glass} \quad (4)$$

$$HVL = \frac{\ln(2)}{LAC} = \frac{0.693}{LAC} \quad (5)$$

$$MFP = \frac{1}{LAC} \quad (6)$$

The value of the effect atomic number ( $Z_{eff}$ ) in Eq. (9) was calculated using the value of the atomic cross section ( $ACS$ ) calculated by Eq. (7) and the effective atomic number (ECS) derived from Eq. (8).

$$ACS = \frac{MAC}{N_A \sum \frac{w}{A}} \quad (7)$$

$$ECS = \frac{1}{N_A} \left( \sum \frac{f \cdot A}{Z} \cdot (MAC) \right) \quad (8)$$

$$Z_{eff} = \frac{ACS}{ECS} \quad (9)$$

where  $w$ ,  $f$ ,  $Z$ ,  $A$  are the weight fraction of the element, the fraction of abundance of the element, the atomic number of the element, and the atomic weight of a constituent element, respectively.

Then, the percentage of relative difference ( $RD$ ) of the results obtained from software Phy-X and XCom was calculated using Eq. (10).

$$RD = \frac{MAC_{XCom} - MAC_{Phy-x}}{MAC_{XCom} + MAC_{Phy-x}} \times 100 \quad (10)$$

Here,  $MAC_{XCom}$  stands for the  $MAC$  result obtained from software XCom and  $MAC_{Phy-x}$  refers to the  $MAC$  results obtained from software Phy-X.

## 2.5 Optical Properties Measurements

Optical absorbance spectrum of glass samples was measured in the wavelength range of 200 to 1100 nm using ultraviolet-visible (UV-VIS) spectrophotometer UV-3600i Plus from Shimadzu. The absorbance ( $A$ ) values were used to calculate the absorption coefficient ( $\alpha$ ) using the following Eq. (10).

$$\alpha = 2.303 \frac{A}{t} \quad (11)$$

where  $t$  indicates the thickness of glass samples.

Tauc's plot, a graph of  $(\alpha hv)^{1/2}$  vs  $(hv)$  was then used to determine the value of  $E_{opt}$  where the  $E_{opt}$  value can be determined by the x-intercept of the Tauc's plot. Then, to determine the value of molar polarizability ( $\alpha_m$ ) as shown in Eq. (13) refractive index ( $n$ ) and molar refraction ( $R_m$ ) value was calculated using Eq. (11), and Eq. (12), respectively.

$$n = \sqrt{-2 + \frac{3}{\sqrt{\frac{E_{opt}}{20}}}} \quad (12)$$

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

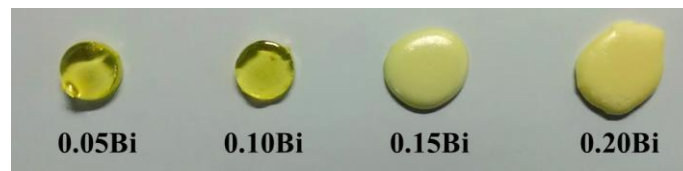
$$\alpha_m = \frac{3}{4} \left( \frac{R_m}{\pi N_A} \right) \quad (14)$$

where  $\pi$  stands for the value of pi, and  $N_A$  refers to Avogadro's constant.

### 3. Results and Discussions

#### 3.1 Glass Composition, Density, and Molar Volume

Figure 1 shows the fabricated glass samples and ceramic samples. The fabrication of the glass samples was stopped at 0.10Bi glass since further incorporation of  $\text{Bi}_2\text{O}_3$  caused the samples to turn opaque. The opaque nature of 0.15Bi and 0.20Bi ceramics was due to their compact structure which resulted from the excessive incorporation of high-density  $\text{Bi}_2\text{O}_3$ . This caused UV and infrared light unable to transmit through the material causing the material to appear opaque. As for 0.05Bi and 0.10Bi glass, visible light waves were able to transmit through the glass leading to transparent glass. Then, the observed yellowish color of the glass samples is due to the incorporation of  $\text{Tm}_2\text{O}_3$ . The formation of defects in the glass network caused the formation of color centers. These color centers caused glass to absorb and emit specific wavelengths of light [23]. Thulium has an emission wavelength at peaks 458nm, 470 nm, and 650nm where energy transition  $^1\text{D}_2$  to  $^3\text{F}_4$ ,  $^1\text{G}_4$  to  $^3\text{H}_6$ , and  $^1\text{G}_4$  to  $^3\text{F}_4$ , respectively occur [24]. This thulium emission wavelength correlates with yellow color emission wavelength which is in the range of 500nm to 650nm [25]. This proved the influence of thulium which caused the visible yellow color of the glass.



**Fig. 1.** Fabricated thulium doped bismuth tellurite glass and ceramics

Table 1 summarizes the fabricated samples' chemical composition, molar mass, density, molar volume, oxygen packing density (*OPD*) and color of fabricated samples. The molar mass of the samples increases as the mol % of  $\text{Bi}_2\text{O}_3$  incorporated increases. This is due to heavy metal bismuth (Bi) atoms that replace other lighter atoms. Also, the density of the samples increases as the mol % of  $\text{Bi}_2\text{O}_3$  incorporated increases indicating that a stronger glass network connectivity was formed [26]. Theoretically, the relationship between density and molar volume should be inversely proportional as shown in Eq. (2). However, the molar volume of the fabricated glass increases as the density increases. This indicates the number of non-bridging oxygens (NBOs) reduces in the glass network. The reduction of NBOs was confirmed further by the calculation of *OPD*. It was found that the *OPD* increases as the mol % of  $\text{Bi}_2\text{O}_3$  increases indicating  $\text{Bi}_2\text{O}_3$  acts as a network former. However, when  $\text{Bi}_2\text{O}_3$  was added excessively in 0.15Bi and 0.20Bi, the samples turned opaque as shown in Figure 1. When there is too much network in the glass structure, it could block visible light. Thus, only 0.05Bi and 0.10Bi will be characterized further for transparent radiation shielding glass for medical and industrial applications.

**Table 1**

Sample code, chemical composition, molar mass, density, molar volume, oxygen packing density and color of thulium doped tellurite glass

Sample Code	Chemical Composition (mol %)			Molar Mass (g/mol)	Density (g/cm <sup>3</sup> )	Molar Volume (cm <sup>3</sup> /g)	Oxygen Packing Density (g/cm <sup>3</sup> )	Color
	TeO <sub>2</sub>	Bi <sub>2</sub> O <sub>3</sub>	Tm <sub>2</sub> O <sub>3</sub>					
0.05Bi	93	5	2	179.44	5.45	32.998	62.731	Transparent Light-yellow
0.10Bi	88	10	2	194.76	5.91	32.938	64.364	Transparent Light- yellow
0.15Bi	83	15	2	210.08	6.41	32.789	66.181	Opaque yellow
0.20Bi	78	20	2	225.40	6.55	34.422	64.493	Opaque yellow

A comparison between the density of fabricated glass samples with lead-based radiation shielding material is shown in Table 2. It is clearly shown that the fabricated glass samples have much higher density than lead glass. This proves the applicability of the glass to be used in industry.

**Table 2**

Glass code, chemical composition, density, and molar volume of thulium doped tellurite glass

Glass	Density (g/cm <sup>3</sup> )
0.05Bi (This work)	5.45
0.10Bi (This Work)	5.91
(Li <sub>2</sub> O) <sub>10</sub> (PbO) <sub>30</sub> (Bi <sub>2</sub> O <sub>3</sub> ) <sub>10</sub> (B <sub>2</sub> O <sub>3</sub> ) <sub>50</sub> [27]	4.93
(Li <sub>2</sub> O) <sub>10</sub> (PbO) <sub>30</sub> (B <sub>2</sub> O <sub>3</sub> ) <sub>60</sub> [27]	4.38
(Na <sub>2</sub> O) <sub>10</sub> (Quartz) <sub>60</sub> (PbO) <sub>30</sub> [28]	4.70
RS 323 G19 Schott Glass (33% lead) [29]	3.26
RS 360 Schott Glass (45% lead) [29]	3.60
RS 520 Schott Glass (71% lead) [29]	5.18

### 3.2 Structural Properties

FTIR analysis was conducted to evaluate the structural bonds that are present in the fabricated thulium-doped bismuth tellurite glass. Figure 2 shows the FTIR spectrum and Table 3 describes the assignment of transmission peaks observed at specific wavenumber. The appearance of the transmittance peak at 622 cm<sup>-1</sup> wavenumber indicates the stretching vibration of stretching vibrations of TeO<sub>4</sub> structural units [30]. Meanwhile, the presence of Te-O bonds of TeO<sub>3</sub> structural units is indicated by the transmittance peak at 704 cm<sup>-1</sup> [31,32]. This shows that tellurite is made of TeO<sub>n</sub> where n = 4, 3+1, and 3 [33]. The variation of structural units is due to local inhomogeneity whereby electrons do not transfer the glass modifier atoms to all the structural units [34]. In this case, the modifier atoms are Bi. Hence, in the fabricated glass consists of three states of tellurite structural units. However, the structural bonds of Bi-O cannot be observed due to instrument limitations where high noise was observed at a wavenumber lower than 600 cm<sup>-1</sup> [35]. The Bi-O bonds should be observed at wavenumber 50 cm<sup>-1</sup> to 500 cm<sup>-1</sup>. Furthermore, the presence of a sharp peak at 1214 cm<sup>-1</sup> indicates the bending of water molecules H<sub>2</sub>O or/and the overtone of O–Te–O symmetric stretch [36]. Then, the sharp peaks at 1368 cm<sup>-1</sup> and 1740 cm<sup>-1</sup> were attributed to the stretching mode of weak Te–OH and strong Te–OH structural bonds. Notice that the intensity of the peaks at wavenumbers 1214 cm<sup>-1</sup>, 1368 cm<sup>-1</sup> and 1740 cm<sup>-1</sup> appear shaper in 0.05Bi glass than 0.10Bi glass. This indicates the incorporation of a glass modifier which in this case Bi<sub>2</sub>O<sub>3</sub> reduces the weak hydrogen bonds of Te-OH [36]. Then, the presence of small peaks at 2076 cm<sup>-1</sup> and 2286 cm<sup>-1</sup> was due to O-H bond bending while a small peak at 3000 cm<sup>-1</sup> was due to O-H bond stretching. These O-

H bond bending and stretching were assigned to water molecules type 1 H<sub>2</sub>O(I) which were probably trapped in the glass network with restricted motion [37,38]. Based on the FTIR result, the peak for a Tm-O bond was not observed. The peak could not be detected since the concentration of Tm<sub>2</sub>O<sub>3</sub> incorporated in the glass composition was very low. A similar result was also observed by Hasnimulyati *et al.*, [39]. However, the presence of thulium can be verified by colour centre as discussed in section 3.1.

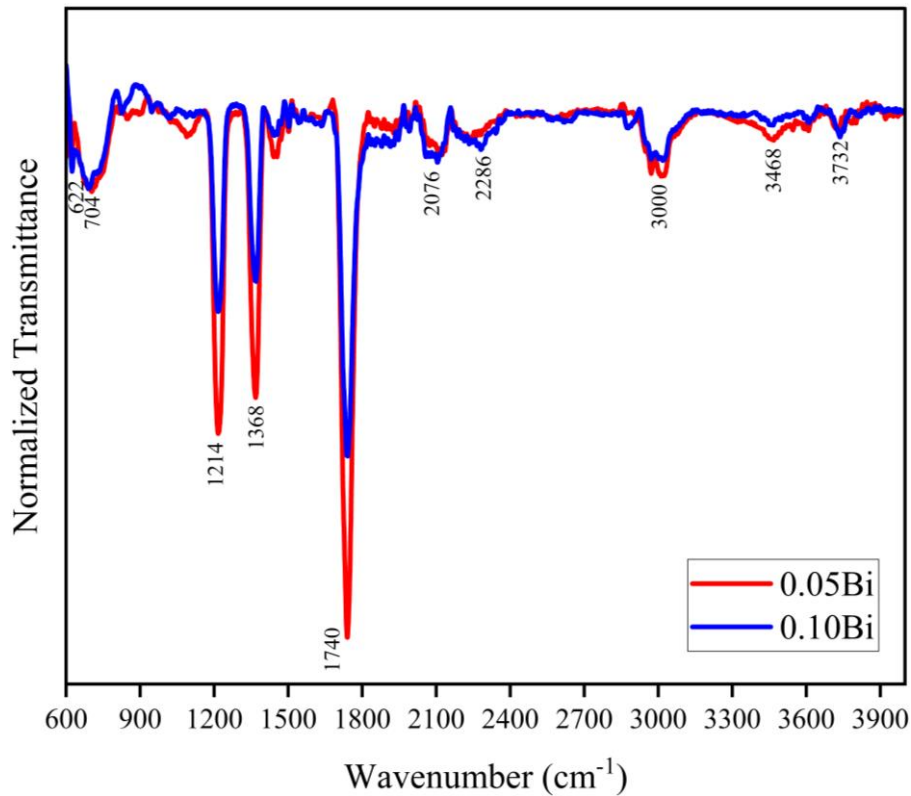


Fig. 2. FTIR spectrum of thulium doped bismuth tellurite glass

Table 3

FTIR structural properties investigation of thulium doped tellurite glass

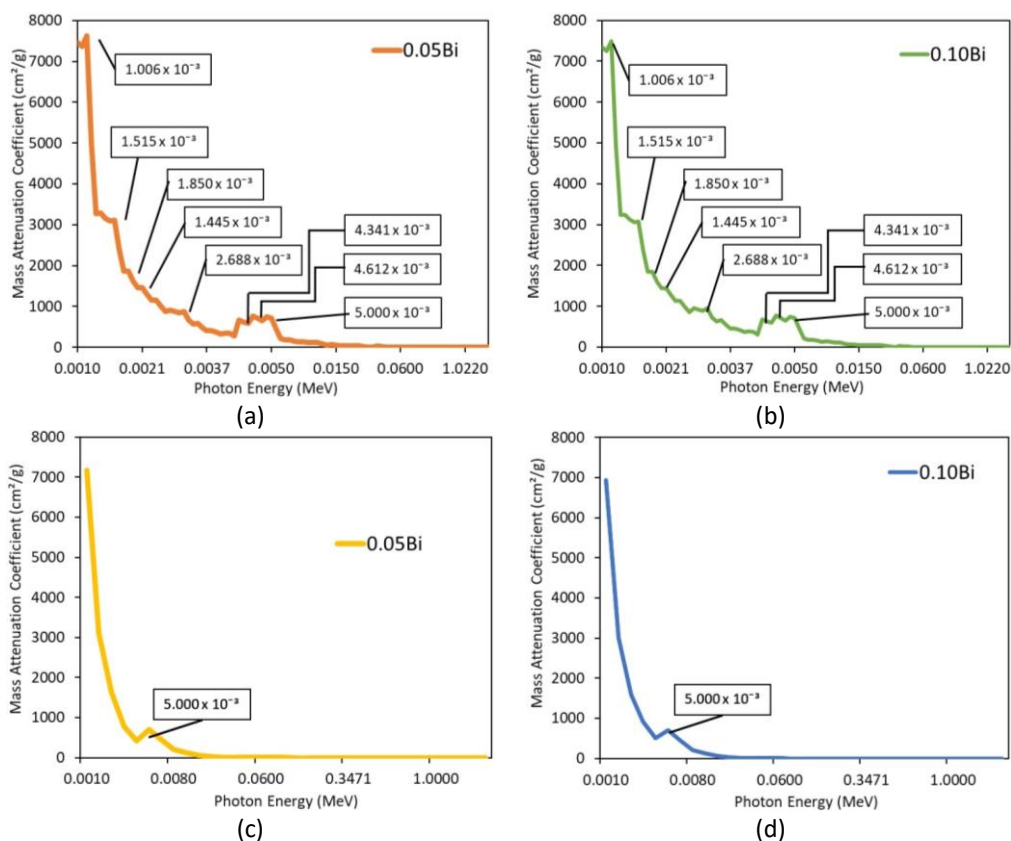
Wavenumber (cm <sup>-1</sup> )	Assignment	Ref.
622	Stretching vibrations of TeO <sub>4</sub> structural units	Gupta <i>et al.</i> , [30]
704	Stretching vibrations of TeO <sub>3</sub> / TeO <sub>3+1</sub> structural units	Kaur <i>et al.</i> , [31] He <i>et al.</i> , [32]
1214	Overtone of O–Te–O symmetric stretch and/or bending mode of molecular water	Cheng <i>et al.</i> , [36]
1368	Weak Te–OH bonds stretching	Cheng <i>et al.</i> , [36]
1740	Strong Te–OH bonds stretching	Cheng <i>et al.</i> , [36]
2076	O–H bonds bending vibration of water molecules in glasses	Brokmann <i>et al.</i> , [37]
2286		
3000	O–H stretching of water molecule in glasses	Brokmann <i>et al.</i> , [37]

### 3.3 Radiation Shielding Properties

The interaction of photons and radiation shielding material can be observed based on the result of the mass attenuation coefficient (*MAC*). Based on Figure 3 *MAC* showed dependency on photon energy where photon interactions such as the photoelectric effect, Compton scattering and pair-production occurred within the attenuated glass. As shown in Figure 3(a) and Figure 3(b), at low

energy levels (0.001 MeV to 0.004 MeV), rapidly decreased of *MAC* was due to the interaction of the photoelectric effect became dominant [40]. Then, at the intermediate energy level where 0.004 MeV to 0.013 MeV for software XCom in Figure 2(a) and 0.004 MeV to 0.015 MeV for software Phy-X in Figure 2(b), the slower decrease of *MAC* was due to the interaction of Compton scattering [41]. At high energy which is above 0.013 MeV for software XCom and 0.015 MeV for software Phy-X, the *MAC* is an almost constant curve indicating the pair production interaction of photons [42].

Based on the result of *MAC* obtained from software XCom, a few sudden sharp peaks are observed in Figure 3(a). These sharp peaks are due to the absorption edge phenomena. The absorption edge phenomena occur when the absorbed photon energy corresponds to the electronic transition or ionization potential of atoms. The absorption edge peak indication was obtained directly from the software XCom. The Te atoms caused a sudden peak at  $1.006 \times 10^{-3}$  MeV due to the M-absorption edge. Meanwhile, the sharp peaks at  $1.515 \times 10^{-3}$  MeV,  $1.850 \times 10^{-3}$  MeV, and  $1.445 \times 10^{-3}$  MeV were caused by the M-absorption edge of Tm atoms. Then, a peak at  $2.688 \times 10^{-3}$  MeV was attributed to the M-absorption edge of Bi atoms. Three distinguished peaks at  $4.341 \times 10^{-3}$  MeV,  $4.612 \times 10^{-3}$  MeV, and  $5.000 \times 10^{-3}$  MeV were due to the L-absorption edge of Te atoms. However, as for *MAC* results obtained from software Phy-X in Figure 3(b), the only distinguishable sharp peak only observed at  $5.000 \times 10^{-3}$  MeV. This sharp peak was due to the L-absorption edge of Te atoms.



**Fig. 3.** Mass attenuation coefficient of thulium doped bismuth tellurite glass at different photon energies obtained from software (a) XCom for 0.05Bi glass, (b) XCom for 0.10Bi glass, (c) Phy-X for 0.05Bi glass, and (d) Phy-X for 0.10Bi glass

The percentage of relative difference (RD) of *MAC* for software Phy-X and XCom is 1.93% for 0.05Bi glass and 3.08% for 0.10Bi glass as shown in Table 4. This low RD indicates that good detection system of the software [43]. The percentage difference was due to systematic error where a different



method was applied for stoichiometric calculation. For software Phy-X, the density of the glasses used for simulation was obtained through an experimental method while software XCom calculated the density of the glass samples based on the molar mass and molar volume of the atoms in the compound mixture.

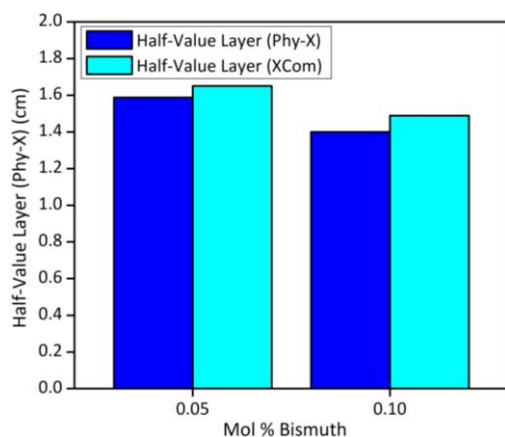
**Table 4**

Glass code, mass attenuation coefficient and percentage relative difference of thulium doped bismuth tellurite glass

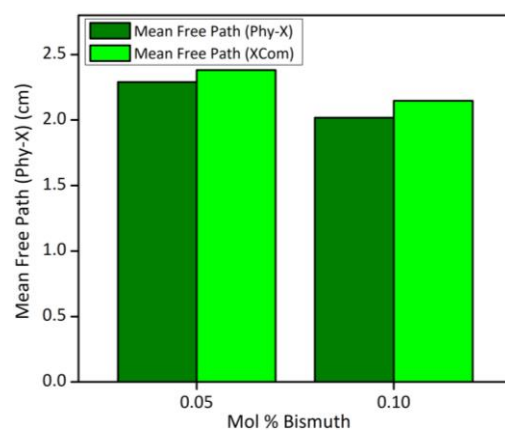
Glass Code	Mass attenuation coefficient at 0.662 MeV (cm <sup>2</sup> /g)		Percentage of relative difference, RD (%)
	Phy-X	XCom	
0.05Bi	0.0801	0.0771	1.93
0.10Bi	0.0838	0.0788	3.08

The half-value layer (*HVL*) of 0.05Bi and 0.10Bi glass was analyzed at photon energy 0.662 MeV. Photon energy released at 0.662 MeV by <sup>137</sup>Cs produced high-energy gamma radiation. This high-energy gamma radiation is currently used in the medical industry especially for cancer treatment as deep tissue penetration can be achieved [44]. Based on the results *HVL* obtained from software Phy-X and XCom in Figure 4, it was found that the glass with 0.10Bi had lower *HVL* than 0.05Bi. Low *HVL* indicates that the material can shield radiation better since the low distance it takes for the harmful radiation rays to reduce to half of its original value.

Figure 5 shows the result of the mean free path (*MFP*) at a photon energy of 0.662 MeV for software Phy-X and XCom. The *MFP* indicates the average distance a unit of radiation can travel in the material before being absorbed. The result depicted that the 0.10Bi glass has a lower *MFP* than 0.05Bi. This low value of *MFP* in 0.10Bi glass indicates that 0.10Bi glass is more efficient at absorbing radiation rays than 0.05Bi glass [45]. A higher concentration of than Bi<sub>2</sub>O<sub>3</sub> in 0.10Bi than 0.05Bi resulted in more photon interaction with radiation shielding glass.



**Fig. 4.** Half-value layer of thulium doped bismuth tellurite glass at photon energy 0.662 MeV for software Phy-X and XCom

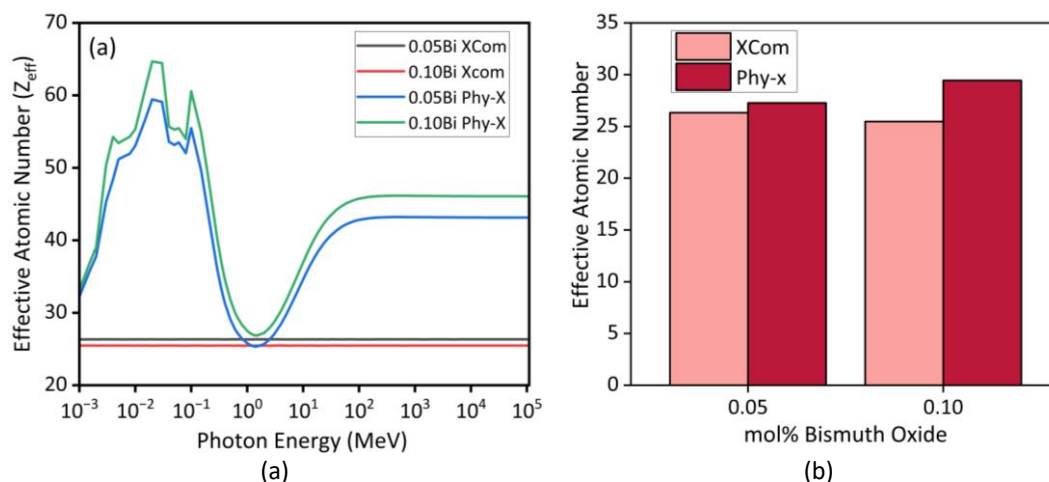


**Fig. 5.** Mean free path of thulium doped bismuth tellurite glass at photon energy 0.662 MeV for software Phy-X and XCom

Figure 6 shows the result of the effective atomic number ( $Z_{eff}$ ) of thulium-doped bismuth tellurite glass. The  $Z_{eff}$  investigation was conducted at continuous energy between 0.001 MeV to 10 000 MeV, and specifically at 0.662 MeV as shown in Figure 6(a), and Figure 6(b), respectively. Significantly, the  $Z_{eff}$  results calculated from software XCom are energy independent while the results simulated from software Phy-X are energy dependent as shown in Figure 6(a). The energy-independent  $Z_{eff}$  from software XCom is close to the calculated value of the composition's mean

atomic number. Similar energy-independent  $Z_{eff}$  was also observed in a study done by Huse *et al.*, [46]. Hence, this shows the limitation of XCom software. Conversely, the energy-dependent  $Z_{eff}$  obtained from software Phy-X makes it possible to evaluate the photon interaction with shielding material.

Similar to *MAC*, a sharp increase of  $Z_{eff}$  at low energy levels was due to the dominant interaction of the photoelectric effect [47]. Meanwhile, a progressive decrease of  $Z_{eff}$  at intermediate energy levels indicates Compton scattering becomes dominant [48]. Then, at high energy levels, pair-production interaction dominance can be portrayed by constant  $Z_{eff}$  curves [49]. It is also observed that there are a few sudden sharp peaks in  $Z_{eff}$  curves due to the absorption edge. A detailed explanation regarding absorption edge was discussed in the *MAC* section. Then, the effect of  $\text{Bi}_2\text{O}_3$  on  $Z_{eff}$  at 0.662 MeV photon energy is shown in Figure 6(b). A high value of  $Z_{eff}$  is favourable since it indicates that a high number of photons attenuated because shielding material has become the preferred target for photons. Thus, photons would collide more frequently with the atoms of shielding material [11]. The 0.10Bi glass results in a higher value of  $Z_{eff}$  at 0.662 MeV photon energy. This is due to the incorporation of bismuth which has a high atomic number causing a high  $Z_{eff}$  value. Bismuth which is a heavy element causes more collision of radiation rays to occur within the glass material [50].

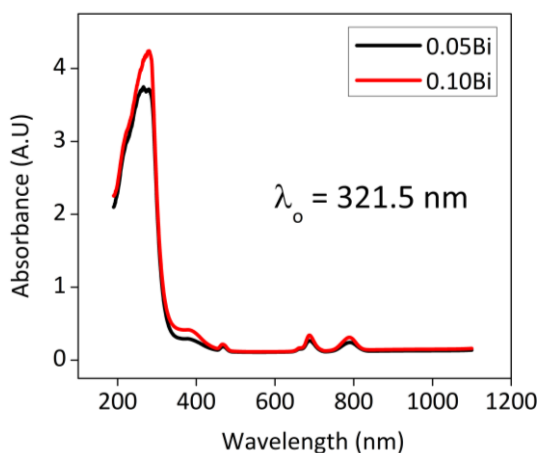


**Fig. 6.** Effective atomic number of thulium doped bismuth tellurite glass at (a) continuous energy range from 0.001 MeV to 10 000 MeV, and (b) photon energy 0.662 MeV for software Phy-X and XCom

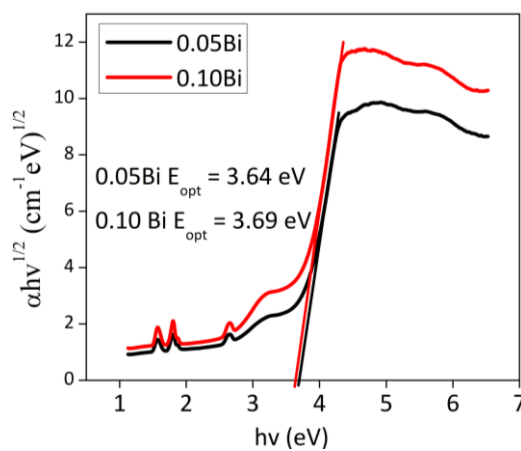
### 3.4 Optical Properties

Figure 7 shows the UV-VIS absorption spectra of 0.05Bi and 0.10Bi glass where the investigated wavelength range is 200 nm to 1100 nm. A dominant central wavelength ( $\lambda_c$ ) was observed at 321.5 nm for both 0.05Bi and 0.10Bi glass. This central wavelength lies in the visible light spectrum. Based on Figure 7, the absorbed light is higher in 0.10Bi glass than 0.05Bi glass indicating the degree of transparency in 0.10Bi glass is lower than 0.05Bi glass [51]. Then, extrapolation of the graph  $(\alpha hv)^{1/2}$  vs  $(hv)$  provides the result of optical band gap ( $E_{opt}$ ) for 0.05Bi and 0.10Bi glass as shown in Figure 8. The  $E_{opt}$  of 0.10Bi glass is higher than 0.05Bi glass due to lower number of NBOs in the glass structure which was proven by *OPD*. The lower NBO number was caused by the incorporation of  $\text{Bi}_2\text{O}_3$  in the glass composition resulting in Te–O–Te or O–Te–O bond bending vibrations drastically decreasing in the FTIR spectrum. This results in a more compact structure that was discussed previously in the density section. Both fabricated glasses also exhibit high transparency which is evidenced by the drop

of  $(\alpha hv)^{1/2}$  vs  $(hv)$  curves at energies less than  $E_{opt}$  [52]. Comparing 0.05Bi and 0.10Bi, the curve of  $(\alpha hv)^{1/2}$  vs  $(hv)$  for 0.05Bi drops more drastically than 0.10Bi at energies less than  $E_{opt}$ . A drastic drop of  $(\alpha hv)^{1/2}$  vs  $(hv)$  indicates a material has high transparency [53].

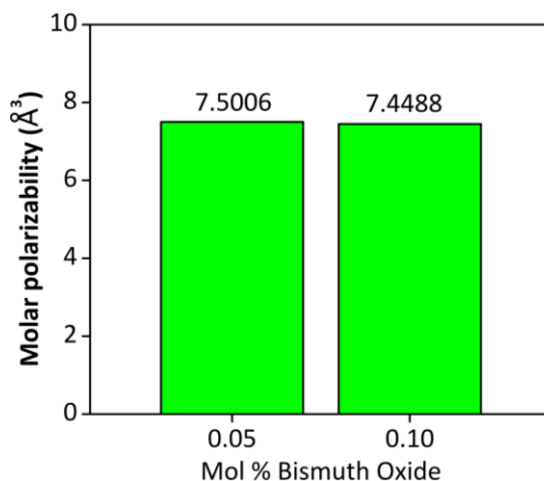


**Fig. 7.** Absorbance spectra of thulium doped bismuth tellurite glass



**Fig. 8.** Tauc's plot graph of  $(\alpha hv)^{1/2}$  vs  $(hv)$  for thulium doped bismuth tellurite glass

Figure 9 shows the molar polarizability of 0.05Bi and 0.10Bi glass. The 0.05Bi glass poses slightly higher molar polarizability compared to 0.10Bi. A high number of NBOs caused molar polarizability to also become high [54]. Compared to bridging oxygens (BOs), nonbridging oxygens (NBOs) have a higher tendency to polarize [55]. In applications that require line-of-sight, polarized glass is desired. Polarized glass could eliminate glare which could partially block humans' vision [56]. When polarized sunglasses were applied in road sports, it was found that polarized sunglasses were able to block glare from direct sunlight and sunlight reflected by the road [57].



**Fig. 9.** Bar graph of molar polarizability thulium doped bismuth tellurite glass

#### 4. Conclusions

In this study, a new composition of  $TeO_2)_{1-x} (Bi_2O_3)_x (Tm_2O_3)_{0.02}$  was successfully fabricated. Structural investigation by FTIR shows the Te–O–Te or O–Te–O bond bending vibrations and Bi–O bonds. Then, a radiation shielding investigation was conducted using the software Phy-X and XCom. Based on the *MAC* results, the interaction of the photoelectric effect, Compton scattering, and pair-

production occur at the same energy range for both glasses due to similar compounds incorporated in the glass composition. The 0.10Bi glass exhibits better radiation shielding capability than 0.05Bi glass. This can be seen based on the result of  $HVL$ ,  $MFP$ , and  $Z_{eff}$ . The 0.10Bi glass has lower  $HVL$  and  $MFP$  as well as higher  $Z_{eff}$  than 0.05Bi glass. However, in terms of optical properties, the 0.05Bi glass performs better than the 0.10Bi glass. This can be depicted based on the result of absorption spectra,  $E_{opt}$  and molar polarizability. The  $E_{opt}$  of the 0.05Bi glass is lower than the 0.10Bi glass due to the high number of NBOs in the glass structure which was proven by the low value of  $OPD$ . Also, the 0.05Bi glass poses slightly higher molar polarizability compared to 0.10Bi. In applications that require line-of-sight, polarized glass is able to eliminate glare which could partially block humans' vision. All in all, both 0.05Bi and 0.10Bi have higher density than the glass containing lead. Therefore, the fabricated glass sample would perform better as radiation-shielding glass compared to lead glass. Hence, this lead-free glass can be widely used in radiation shielding applications that require transparency.

### Acknowledgement

This research was funded by MyBrainSc scholarship and GPJP grant (UPNM/2022/GPJP/SG/3).

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