MoO$_3$-TeO$_2$ glass system for gamma ray shielding applications

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Abstract

This paper examines the gamma-ray shielding features of some selected tellurite-based glasses in the form of xMoO$_3$(100−x)TeO$_2$ (20 ≤ x ≤ 50 mol%). Mass attenuation coefficients (μ$_m$) of these glasses have been calculated using Geant4 toolkit and XCOM program for photon energy range of 1 keV—1000 MeV. The correlation factor (R$^2$) between these two methods was found to be almost one. Shielding effectiveness for these glasses has been estimated by computing half value layer (HVL), effective atomic number (Z$_{eff}$), and mean free paths (MFP). It was noticed that the heavy metal oxide of TeO$_2$ plays an important role in improving the shielding effectiveness of the glasses. The Mo20Te80 glass has shown the promising properties to serve for gamma ray protection applications as compared with many conventional concretes and other newly developed glasses.

1. Introduction

In the field of advanced materials, glasses are promising ones due to their numerous applications as well as their physical and chemical characterizations such as ease of designing, high corrosion resistance, optical transparency, and environment friendly. Previously, many opaque materials such as concrete were suggested as shielding materials for gamma radiation, however, there are several risks and limitations associated with their use [1, 2]. Currently, glasses have the largest interest as promising radiation shielding materials to be used in the windows and doors in medical diagnostic labs, x-ray rooms and CT scans, scintillators, radiation therapy chambers, and in space technology [3, 4]. This triggered an international interest to study many glasses doping with heavy metal oxide (HMO) to serve for various gamma ray shielding applications.

The TeO$_2$ glasses can be used as promising materials for many applications due to their unique structure, physical and optical features [5]. Also, these glasses have a wide range of transparency (400 nm—6 μm), low melting point nature and non-hygrosopic [6]. On the other hand, the significant use of x-ray and gamma-ray in many fields requires hard efforts to search for new materials which are economic, environment friendly, and proper protective against x-ray and gamma-ray. In this regards, several authors reported different type of glasses as promising shielding materials [7–11]. Sayyed [7] proposed some HMO glasses such as PbO, MgO, Ag$_2$O, Nb$_2$O$_5$, ZnO and BaO for gamma-ray applications. It was found that the glasses with PbO have the lowest values of MFP, whereas the glasses with MgO have the highest values of MFP. The results were compared with some concretes. Phosphate glasses were also studied and it was noted that the substitution of ZnO by PbO improves the gamma-ray shielding ability of the glasses [11]. However, the toxicity the lead (Pb) provide strong motivations to replace Pb element by another high−Z element such as Mo, Ba, W, Bi, Gd and etc. Therefore, hard efforts are being put by many authors to find suitable substitute glasses instead of lead to find equivalent shielding properties.

The gamma-ray shielding ability of the materials can be studied by using WinXcom program, experimental measurements or Monte Carlo simulation. These methods depend on Beer–Lambert law that can applied in the case of narrow beam geometry [12, 13]. However, the experimental is restricted to limited photon energies that can not be found easily or cheaply [14–16]. The simulation technique is proposed as a strong alternative to the...
experiment. This technique can handle all the difficulties of the experiment. Monte Carlo simulation is a widespread method to study the interaction of radiation (like gamma) with the matter by providing several models for electromagnetic interactions [17].

The objective of this work is to study the gamma-ray properties of newly developed tellurite-based glasses in the chemical form of $x\text{MoO}_3(100-x)\text{TeO}_2$ ($20 \leq x \leq 50$ mol%) [18]. All the important gamma-ray shielding parameters such as $\mu_m$, HVL, MFP, and $Z_{\text{eff}}$ of these glasses were obtained by using Geant4 toolkit and XCOM program for photon energy $1$ keV—$1000$ MeV. The shielding competence of the present glasses was compared with those of conventional concrete, commercial glasses, and HMO glasses. The data in this work would be helpful to evolve new materials in the gamma-ray protection applications.

2. Materials and methods

Four tellurite-based glasses belonging to the system of $x\text{MoO}_3(100-x)\text{TeO}_2$ with $x = 20, 30, 40,$ and $50$ mol% have been reported to serve for gamma-ray protection applications. The selected glasses (taken from [18]) were coded as Mo20Te80, Mo30Te70, Mo40Te60 and Mo50Te50 for $x = 20, 30, 40,$ and $50$ mol%, respectively. The conventional melt-quenching method was applied to prepare these glasses and Archimedes principle was used to measure their densities [19]. The sample code, density, and nominal composition of the glasses are shown in table 1.

| Sample code | Density (g/cm$^3$) | Compositions (mol%) | Atomic composition (wt.%) |
|-------------|-------------------|---------------------|---------------------------|
|             |                   | MoO$_3$ | TeO$_2$ | O | Mo | Te |
| Mo20Te80    | 5.251             | 20      | 80      | 0.225 | 0.122 | 0.652 |
| Mo30Te70    | 5.176             | 30      | 70      | 0.237 | 0.185 | 0.576 |
| Mo40Te60    | 5.018             | 40      | 60      | 0.250 | 0.250 | 0.499 |
| Mo50Te50    | 4.858             | 50      | 50      | 0.263 | 0.316 | 0.420 |

2.1. Geant4 Monte Carlo simulation

GEANT4 is a radiation propagation Monte Carlo toolkit [17]. This toolkit can be used in numerous fields including high energy physics, astroparticle applications, medical applications, radiation shielding applications [20, 21]. For the radiation shielding studies, GEANT4 offers a wide range of physical models to handle all electromagnetic and nuclear interactions that may occur between the radiation and the shield material.

Figure 1 demonstrates the narrow beam geometry of the GEANT4 simulation, consisting of a point gamma source impinging on a slab of the glass. The gamma photon energies were defined in 662, 1173 and 1332 keV. The thickness of the glass was ranging from 0.1—1 cm according to the gamma-ray energy. Two collimator, one is put after the gammm source and the other is kept before the detector, were also used to focus a beam and ensure that the gamma-rays travel parallel to the collimators. Also, the glass samples were modeled with respect to their atomic number, mass number, elemental weight fractions, and their densities. In this work, one million photons were gunned from monoenergetic source to hit a target of the glass sample. Then, the transmitted photons have been recorded by using sodium iodide (NaI) detector. The $\mu_m$ values of the studied glasses were then calculated.
according to Beer–Lambert law [21, 22]. Moreover, the theoretical values of $\mu_m$ for these glasses were obtained by using XCOM software [23].

2.2. Effective atomic number ($Z_{eff}$)

The $Z_{eff}$ signifies partial photon interactions with the shielding material. The $Z_{eff}$ can be directly calculated by using the relation below [24, 25]:
where \( f_i \) refers to the fractional abundance, and \( A_i \) is the atomic weight. Then, electron density (\( N_{\text{eff}} \)) can be calculated by the equation below [20]:

\[
N_{\text{eff}} = N_i \frac{n Z_{\text{eff}}}{\sum p_i A_i} \quad \text{(electrons/g)}
\]
2.3. Half value layer \((HVL)\)

The HVL is a certain thickness of certain shielding material necessary to reduce gamma-ray intensity to half of its original value. The HVL depends on the energy of gamma-ray and on the type of the shielding material. The following relation gives the numerical value of HVL \([7, 26]\):

\[
HVL = \frac{\ln(2)}{\mu}
\]  

(3)

2.4. Mean free path \((MFP)\)

The MFP is defined by the distance travelled between two gamma-ray collisions. The MFP depends also on the energy of gamma-ray and on the type of the shielding material. The following relation gives the numerical value of MFP \([27]\):

\[
MFP = \frac{1}{\mu}
\]  

(4)

3. Results and discussion

The mass attenuation coefficients of the tellurite glasses in the form \(x\text{MoO}_3(100-x)\text{TeO}_2\) with \(x = 20, 30, 40, \) and 50 mol\% have been determined by using Geant4 toolkit and XCOM software. The obtained results of \(\mu_m\) have been plotted in the energy range of 1 keV–1000 MeV as shown figure 2.

It can be seen that the \(\mu_m\) values of the present glasses depend on the energy of gamma-ray as well as on the atomic composition of the glass sample. The values of \(\mu_m\) were observed to be large when the photon energy is small as well as when the Te content is considerable in the glass sample. When the photon energy is small (0.001–0.5 MeV), one can notice a considerable decrease in \(\mu_m\) values due to the dominance of the photoelectric
absorption process in this energy range. By increasing the photon energy (0.5–4 MeV), the decrease is still in the values of $\mu_m$ but in this case a slight descrease was observed due to the Compton effect. By more increase in the photon energy (4–1000 MeV), a very trivial increase can be seen in the values of $\mu_m$ due to the process of creation and annihilation of electron-positron pairs. Moreover, some abrupt discontinuities can be seen in the figure 2 due to the photoelectric effect near the absorption K-edge of Mo and Te elements at 20 keV and 31.8 keV, respectively. Among our proposed glasses, the one coded as Mo20Te80 have a higher $\mu_m$ due to the Mo20Te80 has higher weight fraction of the heavy metal oxide (TeO2, 80 mol%). The present glasses offer very large $\mu_m$ comparing to commercial glasses [28]. In order to confirm the accuracy of the present $\mu_m$ values, we carried out the Geant4 simulations at some photon energies such as 662, 1173, and 1332keV. The comparision of $\mu_m$ values obtained by Geant4 and XCOM codes is shown in figure 3.

From this figure it is seen that there is strong correlation between the theoeretical and simulation values. Such that we found the correlation factor ($R^2$) of the $\mu_m$ values to be almost one. The calculated $\mu_m$ values were then used to compute $Z_{eff}$ values which were plotted in figure 4.

Obviously, the $Z_{eff}$ values are large at the low energies, small at the intermediate energies, and constant at the high energies. Also, there is an abrupt change occurs at 20–32 keV due to the absorption edges of Mo and Te elements. Moreover, the highest $Z_{eff}$ value was found for Mo20Te80 glass and the lowest $Z_{eff}$ value was noted for Mo50Te50 glass. This is because of that the interaction of photon with matter is directly related to $Z$ (atomic number). For example, the photoelectric interactions rely on $Z^4$, the Compton interactions rely on $Z$, and the pair production interactions rely on $Z^2$. Thus, the highest value of $Z_{eff}$ was noted for Mo20Te80 glass, which contains the highest weight fraction of Te. Since a higher $Z_{eff}$ refers to a better shield against gamma-rays, Mo20Te80 is found to be a superior shielding material among the studied glass samples. The $Z_{eff}$ values of the studied glasses were compared with different promising tellurite glasses in table 2.

Figure 6. MFP of the MoO3-TeO2 glasses compared with other tellurite glasses: (a) Pb20Te80 [7], (b) Mn20Te80 [34], (c) Ti2V48Te50 [29], and (d) Mo20Bi10Te70 [19].
It is clear that the Z_{eff} values of the studied glasses are higher than those of 90TeO_2-10V_2O_5 [29] and 60TeO_2-10B_2O_3-10MoO_3-10ZnO-10Na_2O [30]. On the other hand, the Z_{eff} values of the studied glasses are lower than those of 90TeO_2-10Bi_2O_3 [26], and comparable with those of 80TeO_2-20BaO [27].

The HVL values of the present glasses were calculated and then plotted along with those of ordinary concrete, barite concrete and marble concrete in figure 5. In gamma-ray applications, the lower HVL values indicate to the higher shielding ability of the materials. From figure 5, it can be seen that the HVL values of the present glasses are very small at the low photon energies. Then, HVL values increase as the photon energy increases and a peak was observed around 10 MeV for all studied glasses. Thereafter, the HVL values of the present glasses decrease with increasing the photon energy. Such behavior of HVL values with incident photon energy can be explained similarly to the aforementioned discussion of μ_{ia}. The HVL values of the MoO_3-TeO_2 glasses were compared with those of different types of concrete; (a) Ordinary concrete [31], (b) Barite concrete [32], and (c) Marble concrete [33]. It is seen obviously that the shielding properties of the present glasses are better than those of conventional concrete and thus these glasses can serve as shielding materials for gamma-rays applications. The MFP values of the studied glasses are calculated and then plotted along with those of collected tellurite glasses in figure 6.

The MFP values of the studied glasses were observed to be low at the low energies. By the increasing of the photon energy the MFP values increase very fast, so in the shielding applications it is better to increase the thickness of the glass because the gamma-ray can penetrate the glass more deeply. Moreover, figure 6 reveals that the present glasses have better shielding properties than those of Ti_2V_48Te_50 glass [29], lower than those of Pb_20Te_80 [7] glass and comparable with those of Mn_20Te_80 [34] and Mo_20B_10Te_70 glasses [19].

4. Conclusion

In the present work, four glasses belonging to the system of xMoO_3(100-x)TeO_2 (20 ≤ x ≤ 50 mol%) have been investigated for gamma-shielding applications. The μ_{ia} values of these glasses were obtained by Geant4 Monte Carlo simulation and by XCOM program. The Monte Carlo simulation and XCOM results were comparable. The shielding effectiveness parameters such as Z_{eff}, HVL and MFP were computed. The presence of TeO_2 reduces MFP values and improves the gamma-ray shielding effectiveness. Mo_20Te_80 glass was found to be most promising shielding materials as compared with many conventional concretes and other newly developed glasses.

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