Bonginkosi Vincent Kheswa*

X-ray shielding properties of bismuth-borate glass doped with rare earth ions

Abstract: In this study, the X-ray shielding competence of the 15Bi2O3 + 75H3BO3 + 10Sm2O3, 15Bi2O3 + 75H3BO3 + 10Nd2O3, and 15Bi2O3 + 75H3BO3 + 10CeO2 glasses was investigated using the Phy-X/PSD simulation software and validated using the XCOM simulation software. The Sm3+ doped bismuth-borate glass gave the highest linear attenuation coefficients and effective atomic number, and the lowest half-value layer, tenth-value layer, and mean free path. Thus, it is the most effective radiation shielding material compared to the Nd3+ and Ce4+ doped bismuth-borate glasses. It was also observed that the Sm3+ doped bismuth-borate glass also has better radiation-shielding competence than various glass systems that have been recently investigated in the literature.

Keywords: bismuth-borate glass, X-ray shielding, Sm3+, Nd3+, Ce4+

1 Introduction

X-rays are an ionizing radiation that has a typical energy range of hundred eV to hundreds of keV. X-rays can be produced as characteristic X-rays or bremsstrahlung radiation. They are used in various industries for numerous applications. For instance, in medicine, they are used for mammography, dental X-rays, computed tomography scans, and fluoroscopy. In security, they are used for screening freight trains, containers, automobiles, and luggage. They are also used for the maintenance and repair of oil and gas supply pipelines in power plants. In the food industry, they are used to detect odd objects. In all these applications, X-rays pose health risks to humans if they are not well shielded.

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Graphic abstract: X-rays are an ionizing radiation that is used in various industries such as the food industry, nuclear research facilities, nuclear power plants, radiography, dentistry, and gas supply pipeline maintenance. Exposure to this radiation poses health risks to humans. As a result, it is vital to shield them as much as possible. This can be performed using numerous materials that have high density and high X-ray attenuation coefficients. Metallic lead and concrete are the conventional materials that have been used for shielding X-rays in hospitals and nuclear facilities. However, lead is very toxic to humans, and it is no longer preferred in radiation shielding. The disadvantage of concrete is that it is not transparent. As a result, different researchers have been developing heavy-element based glasses and testing their radiation-shielding competence so that they can be used as an alternative to lead and concrete. A few years ago, new bismuth-borate glasses, which are doped with Sm3+, Nd3+, and Ce4+, were developed. Their X-ray shielding properties were simulated, in this work, using the Phy-X/PSD software and verified using the XCOM software. The results show that the Sm3+-doped bismuth-borate glass is, by far, the most effective radiation-shielding glass compared to the Nd3+ and Ce4+ doped glasses. This is illustrated with the figure above, which depicts the linear attenuation coefficient of the three glasses in the photon energy range of 30–300 keV. In this figure, SSm, SNd, and SCE refer to the Sm3+, Nd3+, and Ce4+doped bismuth-borate glasses, respectively. Furthermore, it is interesting to note that the SSm glass is also more effective than 15Bi2O3 + 10Li2O + 10ZnO + 10GeO2 + 55TeO2 glass, which was found to be the most effective sample in one of the recent studies in the literature.
Various materials can be used to shield X-rays, but the use of metallic lead (Pb) is the most traditional method in hospitals, nuclear research facilities, and the manufacturing industry [1,2]. This is because of the high density and high linear attenuation coefficient (LAC) of Pb. However, lead is very toxic to humans and therefore not user-friendly for radiation shielding [1]. As a result, different researchers have been searching for alternative materials that pose no health risks and have high radiation attenuations [3–12]. The radiation shielding competence of different borate glasses has been studied by various researchers in the X-ray energy region. For example, the impact of Bi$_2$O$_3$ concentration on X-ray shielding properties of TeO$_2$–Li$_2$O–GeO$_2$–ZnO–Bi$_2$O$_3$ glass was recently investigated using Phy-X/PSD software in the 30–300 keV energy range [2]. The results showed that the radiation shielding competence of this glass improves with an increase in the Bi$_2$O$_3$ concentration. Similarly, the radiation shielding properties of Li$_2$O–B$_2$O$_3$–MgO–Er$_2$O$_3$ glasses co-doped with Sm$_2$O$_3$ were investigated, and they were found to greatly improve, in the X-ray energy region, with the increase in the Sm$_2$O$_3$ content [14]. In the same vein, La$_2$O$_3$–CaO–B$_2$O$_3$–SiO$_2$ has been studied and its X-ray shielding capacity increased with the increase in La$_2$O$_3$ concentration [15].

A few years ago, the novel bismuth-borate glasses doped with rare earth Ce$^{4+}$, Nd$^{3+}$, and Sm$^{3+}$ were synthesized and evaluated for their luminescence properties [16]. Recently, these materials were also investigated for optical and γ radiation shielding properties at energies above 284 keV [17]. However, these materials have never been investigated for their X-ray shielding properties in energies below 284 keV, and this is the main focus of this article. The X-ray applications such as airport security, mammography, computed tomography, and X-ray crystallography use X-rays with energies below 284 keV. Hence, it is important to understand X-ray shielding in this energy region in order to improve the protections of humans, involved in the aforementioned applications, from potential radiation hazards. Thus, in this work, the X-ray shielding properties of 15Bi$_2$O$_3$ + 75H$_3$BO$_2$ + 10Sm$_2$O$_3$, 15Bi$_2$O$_3$ + 75H$_3$BO$_2$ + 10Nd$_2$O$_3$, and 15Bi$_2$O$_3$ + 75H$_3$BO$_2$ + 10CeO$_2$ were investigated and discussed in detail. In particular, the LAC, mass attenuation coefficient (MAC), half-value layer (HVL), tenth-value layer (TVL), mean-free path (MFP), and effective atomic number ($Z_{eff}$) of these three glasses were simulated using Phy-X/PSD software in the 30–300 keV X-ray energy region. The results were also validated using the XCOM software.

## 2 Methods

The X-ray shielding capacity of 15Bi$_2$O$_3$ + 75H$_3$BO$_2$ + 10Sm$_2$O$_3$, 15Bi$_2$O$_3$ + 75H$_3$BO$_2$ + 10Nd$_2$O$_3$, and 15Bi$_2$O$_3$ + 75H$_3$BO$_2$ + 10CeO$_2$ were computed using the Phy-X/PSD online software [18,19].

The summary of the samples’ codes, chemical contents, and densities used in this study is shown in Table 1. Phy-X/PSD is a user-friendly software for the calculation of LAC, MAC, HVL, TVL, MFP, $Z_{eff}$, and many more. This software works for all photon energies between 1 keV and 100 GeV. It requires primary input data, which is the chemical composition and density of each sample for which the aforementioned quantities need to be calculated. The chemical composition is required as a mole fraction or weight fraction. The input data used in the Phy-X/PSD calculations are shown in Table 1.

The LAC and MAC describe the interaction probability between X-rays and an absorber material. The higher the LAC and MAC, the better the X-ray shielding capacity of the material. LAC ($\mu$) is calculated using the well-known Beer–Lambert law, which relates the photon counts to the thickness of an absorber according to the following formula:

$$N_f = N_i e^{-\mu t},$$

where $N_i$ and $N_f$ are the photon counts before and after passing through the absorber with thickness $t$, respectively. MAC is calculated from LAC, $\mu$, and material density, $\rho$, as follows [18]:

$$MAC = \frac{\mu}{\rho} = \sum w_i(\mu/\rho)_i,$$

where $w_i$ is the weight fraction of the $i$th constituent element. The HVL and TVL are the thicknesses, of a radiation shielding material, needed to reduce the intensity of X-rays by 50 and 90%, respectively. The lower the HVL and TVL, the better the radiation shielding ability of the material. The HVL and TVL are computed using the LAC according to the following formulas [18]:

$$HVL = \frac{\ln 2}{\mu},$$

$$TVL = \frac{\ln 10}{\mu}.$$
and
\[ \text{TVL} = \frac{\ln 10}{\mu}, \]  
where \( \mu \) is the LAC of the material. Furthermore, the MFP, which is the mean distance required to attenuate photons in an absorber, is calculated from the LAC, \( \mu \), as follows [18].
\[ \text{MFP} = \int_0^{\infty} \frac{te^{-\mu t}dt}{e^{-\mu t}dt} = \frac{1}{\mu}. \]  

The lower the MFP, the better the radiation shielding capacity of the absorber. \( Z_{\text{eff}} \) is also used to assess the superiority of a radiation shielding material. The higher the value of \( Z_{\text{eff}} \), the better the material is in shielding X-rays. The values of the \( Z_{\text{eff}} \) are given by ref. [18]:
\[ Z_{\text{eff}} = \sum f_i A_i \frac{Z_i}{\rho_i}, \]  
where \( f_i \), \( A_i \), and \( Z_i \) are, respectively, the mole fraction of each element, atomic weight, and atomic number in the absorber material.

The results computed with the Phy-X/PSD software were compared with the calculations of the XCOM software. The XCOM software is an online software for the simulation of MAC for photon energies in the 1 keV to 100 GeV range [20,21]. The primary input data required in the XCOM software are the chemical compositions. XCOM requires chemical contents in weight fraction, and the XCOM input values used in this study are shown in Table 2.

### 3 Results and discussion

Our findings on the X-ray shielding properties of 15Bi₂O₃ + 75H₃BO₂ + 10Sm₂O₃, 15Bi₂O₃ + 75H₃BO₂ + 10Nd₂O₃, and 15Bi₂O₃ + 75H₃BO₂ + 10CeO₂ are discussed in detail in this section. In particular, we discuss the LAC, MAC, HVL, TVL, MFP, and \( Z_{\text{eff}} \) of each sample and compare them to the literature. Figure 1 shows the LACs of the SSm, SNd, and SCe glasses as a function of X-ray energy in the 30–300 keV energy region. These results show that the LAC decreases fast with an increase in the X-ray energy for all three glass materials. This trend is consistent with the observations in the literature [10,22,23]. It is because this energy region is dominated by the photoelectric absorption component, of the LAC, which decreases sharply with an increase in photon energy. The SSm glass has the highest LAC at all energies, while SCe has the lowest LAC. In detail, it ranges from 1.946 to 122.594 cm⁻¹, 1.660 to 104.007 cm⁻¹, and 1.589 to 100.614 cm⁻¹ for SSm, SNd, and SCe, respectively. There is also a sudden increase in the LAC at 100 keV for all glasses. This is due to the K absorption edge, which enhances the photoelectric absorption.

To validate the Phy-X/PSD software calculations, we compared the LACs obtained using Phy-X/PSD to the ones obtained using XCOM software, for all three glass samples used in this study. The XCOM software is only able to compute MAC, which is converted to LAC using the densities of SSm, SNd, and SCe materials. This comparison is depicted in Figure 2, and clearly, there is a very good agreement between the XCOM and Phy-X/PSD values of the LAC. Thus, we can trust all other observables computed with the Phy-X/PSD software since they are all based on LAC. Hence, the rest of the radiation shielding parameters presented in this study were computed with the Phy-X/PSD software, and there was no need to further compare them with the XCOM-based calculations.

### Table 2: The chemical contents (wt%) of glass samples used in XCOM calculation

<table>
<thead>
<tr>
<th>Code</th>
<th>Bi₂O₃</th>
<th>H₃BO₂</th>
<th>Sm₂O₃</th>
<th>Nd₂O₃</th>
<th>CeO₂</th>
<th>Density (g/cm³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SSm</td>
<td>0.502</td>
<td>0.247</td>
<td>0.251</td>
<td>—</td>
<td>—</td>
<td>7.1</td>
</tr>
<tr>
<td>SNd</td>
<td>0.507</td>
<td>0.249</td>
<td>—</td>
<td>0.244</td>
<td>—</td>
<td>6.1</td>
</tr>
<tr>
<td>SCe</td>
<td>0.575</td>
<td>0.283</td>
<td>—</td>
<td>—</td>
<td>0.142</td>
<td>5.69</td>
</tr>
</tbody>
</table>

![Figure 1: LAC of SSm, SNd, and SCe.](image-url)
The MAC of each glass sample is shown in Figure 3. The MAC shows a decreasing trend with an increase in X-ray energy for all three materials. In particular, it is in the range of 0.279 – 17.683, 0.272 – 17.050, and 0.274 – 17.267 cm²/g for SCe, SNd, and SSm, respectively. It is also clear that at energies between 0.05 and 0.1 MeV, the MAC of SSm is the highest, while at energies below 0.05 MeV and above 0.1 MeV, all three glasses are comparable. Clearly, no one material has the highest or lowest MAC in the whole X-ray energy region. A similar situation has been observed in other studies [24]. It shows that the materials’ densities have a strong impact on making SSm have the highest LAC (see Figure 1) compared to SNd and SCe.

Figures 4 and 5 show the HVL and TVL that were computed for SSm, SNd, and SCe. It is observed that the HVL of SSm remains the lowest in the entire X-ray energy region. Furthermore, the HVL increases with an increase in photon energy. This behavior has been seen in other studies [25,26]. In detail, it increases from 0.006 to 0.356 cm for SSm, 0.007 to 0.418 cm for SNd, and 0.007 to 0.436 cm for SCe. The TVL shows a similar trend that is observed in the HVL. In this case, the values range from 0.019 to 1.183 cm for SSm, from 0.022 to 1.387 cm for SNd, and from 0.023 to 1.449 cm for SCe. They are also the lowest in the entire energy range for the SSm sample.

The variation of the MFP, of our three glass samples, as a function of X-ray energy is depicted in Figure 6. It is clear
that the MFP increases with the increase in photon energy, and SSm is significantly the lowest in the whole X-ray energy region. In particular, the MFP of SSm increased from 0.008 to 0.514 cm, while the MFP of SNd and SCe ranged from 0.010 to 0.603 cm and from 0.010 to 0.629 cm, respectively. This increasing trend of an MFP as a function of photon energy is consistent with the literature [27].

Figure 7 depicts the distribution of the $Z_{\text{eff}}$ for all three glass materials in the 30–300 keV photon energy range. It is observed that the $Z_{\text{eff}}$ has a decreasing trend with an increase in the X-ray energy. The values of $Z_{\text{eff}}$ decrease from 72.21 to 24.67 for SSm, from 72.04 to 24.37 for SNd, and from 73.37 to 23.19 for SCe. SSm is the highest at energies between 40 and 300 keV, while SCe is highest in the 30–40 keV energy range.

Furthermore, the shielding competence of the SSm, SNd, and SCe samples was compared with other glass samples from the literature, in a way similar to the one used in the previous study [28]. In particular, the MFPs of SSm, SNd, and SCe glasses, at 100 and 50 keV, were compared with the MFP of 80TeO$_2$–20Ag$_2$O (20Ag$_2$O) and 80TeO$_2$–20ZnO (20ZnO) from the previous studies [6,29] and PbCl$_2$–TeO$_2$ (P25T75), Bi$_2$O$_3$–PbCl$_2$–TeO$_2$ (B10P20T70), MoO$_3$–PbCl$_2$–TeO$_2$ (M10P20T70), Sb$_2$O$_3$–PbCl$_2$–TeO$_2$ (S10P20T70), WO$_3$–PbCl$_2$–TeO$_2$ (W10P20T70) and ZnO–PbCl$_2$–TeO$_2$ (Z10P20T70) from the previous study [6]. These comparisons are shown in Figures 8 and 9. It is interesting to see, in Figure 8, that the MFP of SSm, SNd, and SCe at 100 keV is lower than the MFP of P25T75, B10P20T70, S10P20T70, W10P20T70, Z10P20T70, 20Ag$_2$O, and 20ZnO glasses, and SSm still remains the lowest.

It is also observed in Figure 9 that at 50 keV, SCe has the highest MFP compared of P25T75, B10P20T70, M10P20T70, S10P20T70, W10P20T70, Z10P20T70, 20Ag$_2$O, and 20ZnO glasses. On the other hand, SSm clearly has the lowest MFP compared to P25T75, B10P20T70, M10P20T70, S10P20T70, W10P20T70, Z10P20T70, 20Ag$_2$O, and 20ZnO at 50 keV.

In Figure 10, the MFP of SSm, SNd, and SCe, at 50 keV, is also compared to the MFP of the 10Li$_2$O + 10ZnO + 10GeO$_2$ + 70TeO$_2$ (BiTe1), 5Bi$_2$O$_3$ + 10Li$_2$O + 10ZnO + 10GeO$_2$ + 65TeO$_2$ (BiTe2), 10Bi$_2$O$_3$ + 10Li$_2$O + 10ZnO + 10GeO$_2$ + 60TeO$_2$ (BiTe3), and 15Bi$_2$O$_3$ + 10Li$_2$O + 10ZnO + 10GeO$_2$ + 55TeO$_2$
(BiTe4) glasses from the previous study [2]. It is also observed that SSm still has the lowest MFP compared to BiTe1, BiTe2, BiTe3, and BiTe4, while SCe remains the highest.

4 Conclusion

The radiation shielding properties of bismuth-borate glasses were simulated using the Phy-X/PSD and XCOM simulation software. In particular, we computed the LAC, MAC, HVL, TVL, MFP, and $Z_{\text{eff}}$ of 15Bi$_2$O$_3$ + 75H$_3$BO$_2$ + 10Sm$_2$O$_3$, 15Bi$_2$O$_3$ + 75H$_3$BO$_2$ + 10Nd$_2$O$_3$ and 15Bi$_2$O$_3$ + 75H$_3$BO$_2$ + 10CeO$_2$. The Sm$^{3+}$-doped glass has the lowest HVL, TVL, and MFP for all X-ray energies below 300 keV, and it has the highest $Z_{\text{eff}}$ for all photon energies between 40 and 300 keV. In particular, its HVL, TVL, MFP, and $Z_{\text{eff}}$ are, respectively, in the ranges of 0.006–0.356 cm, 0.019–1.183 cm, 0.008–0.514 cm, and 72.21–24.67 in the 30–300 keV X-ray energy region. Hence, Sm$^{3+}$-doped glass has the most superior radiation shielding competence compared to the ones doped with Nd$^{3+}$ and Ce$^{4+}$. It is also intriguing to see that the Sm$^{3+}$-doped glass is even more effective in shielding X-rays than many glass systems that

Figure 8: MFP of SSm, SNd, and SCe compared to other glass materials at 100 keV.

Figure 9: MFP of SSm, SNd, and SCe compared to other glass materials at 50 keV.
have been studied in the literature, which are $80\text{TeO}_2-20\text{Ag}_2\text{O}$, $80\text{TeO}_2-20\text{ZnO}$, $\text{MoO}_3-\text{PbCl}_2-\text{TeO}_2$, $\text{Sb}_2\text{O}_3-\text{PbCl}_2-\text{TeO}_2$, $\text{WO}_3-\text{PbCl}_2-\text{TeO}_2$, $\text{ZnO}-\text{PbCl}_2-\text{TeO}_2$, $10\text{Li}_2\text{O}+10\text{ZnO}+10\text{GeO}_2+70\text{TeO}_2$, $5\text{Bi}_2\text{O}_3+10\text{Li}_2\text{O}+10\text{ZnO}+10\text{GeO}_2+55\text{TeO}_2$, which were recently investigated.

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Data availability statement: All data presented in this article are available on request from the author.

Ethical approval: This computational research does not involve humans or animals.

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