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Investigation of the radiation shielding capability of xPbO–(50 − x)BaO–50B_2O_3 glass system using Geant4, Fluka, WinXCOM and comparison of data with the experimental data

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Abstract. In this study, mass attenuation coefficient (μ_m), transmission fractions (T), effective atomic numbers (Z_{eff}) and half-value layer (HVL) of the xPbO–(50 − x)BaO–50B_2O_3 (where x = 10, 20, 30, 40 mol%) glass system have been determined from the Monte Carlo simulations carried out with Geant4 and Fluka simulation toolkits and WinXCOM database software. The calculated results were compared with the experimentally obtained μ_m values of the selected glass in order to validate the Geant4 model of HPGe detector and Fluka model of NaI(Tl) detectors. T, Z_{eff} and HVL shielding parameters of the studied glass system indicate that increase of PbO content from 10 to 40% results in a better shielding behaviour thanks to the high atomic number of lead.

Keywords. Photon attenuation; glasses; Geant4; Fluka; WinXCOM.

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1. Introduction

Advances in the field of materials science have made great contributions to the development of new materials as per the needs of different application fields. For places where shielding against the penetrating gamma radiation is necessary, the materials used must decrease the intensity of incident radiation to an acceptable level to protect humans against the harmful effects of the ionising radiation. Therefore, efforts are going on worldwide to either experimentally or numerically determine the shielding properties of the newly developed materials. Photon attenuation coefficients and transmission fractions of heavyweight concrete containing mineral admixture were determined experimentally by Gokce *et al* [1]. Gamma-ray shielding properties of two natural clay materials from south western Nigeria were calculated by using the high-purity germanium (HPGe) detector [2]. The photon shielding abilities of gadolinium-containing polymeric compounds were computationally measured using the Geant4 and MCNPX codes [3]. Mass attenuation coefficients of different ceramic samples were experimentally determined at 14 different energies using HPGe detector [4]. Shielding capabilities of the Zn–Cd–Sn–Pb quaternary alloys were experimentally evaluated at 511 and 662 keV photon energies by Kaur *et al* [5]. A comparative study of the shielding properties of different steel alloys computationally was performed using Geant4, MCNP, WinXCOM and experimental results [6]. Mass attenuation coefficients of some fatty acids were calculated experimentally using NaI(Tl) detector [7]. The advantages of optical transparency and easy preparation and production make the glasses attractive for the researchers to investigate and explore their shielding properties. Thus, radiation properties of different glass systems have been investigated in the last few years by numerous researchers. Six glass pieces with a composition of PbO–Li_2O–B_2O_3 were prepared by using the melt quenching technique and the shielding properties of the samples were experimentally determined at four different γ-ray energies. The results of the study showed that the increase of PbO content increases the shielding efficiency [8]. The effect of La_2O_3 on the radiation attenuation characteristics of the lanthanum calcium silicoborate glasses is experimentally

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measured at eight different photon energies between 224 and 662 keV. It was reported that the increase of the La_2O_3 concentration results in an increase in the shielding ability of the lanthanum calcium silicoborate glasses [9]. Shielding properties of $80TeO_2$–$5TiO_2$–$(15 - x)WO_3$–xA_nO_m glasses were investigated by using MCNP5 code and WinXCom. The results of this study revealed that using of $5Er_2O_3$ in the places of xA_nO_m significantly increases γ-ray and neutron shielding behaviour [10]. Gamma and neutron shielding capabilities of 20BaO/SrO–$(x)Bi_2O_3$–$(80 - x)$ B_2O_3 (where x is between 10 and 60 mol) glasses have been investigated computationally by using MCNP5 code and WinXCom. It was published that the addition of Bi_2O_3 increases the shielding effects of the glass system. In this comparative study, mass attenuation coefficients (μ_m), transmission fractions (T), effective atomic numbers (Z_{eff}) and half-value layer (HVL) of the xPbO–$(50 - x)$BaO–$50B_2O_3$ glass system (coded as PbBaB) have been computationally determined using the Geant4 and Fluka simulation toolkits and WinXCOM database softaware. The results were compared with the experimentally calculated results.

2. Materials and methods

2.1 *Theoretical background*

Definition and calculation of the γ-ray shielding parameters of diverse materials are given in [5,11,12]. When a beam of γ-ray photons passes through a material, the intensity of the incident beam shall be attenuated according to the Beer–Lamberts law as given in eq. (1).

$$I = I_0 \cdot e^{-\mu \cdot x}, \tag{1}$$

where I_0 and I are the incident and attenuated photon intensities respectively, x (cm) is the thickness of the material and μ (cm^{-1}) is the linear attenuation coefficient of the sample. For each selected energy, the simulations are first carried out without the glass sample placed between the source and the detector to determine the value of I_0. After that, the simulations are repeated with the glass sample placed between the source and the detector with the thickness from 1 to 5 cm with 1 cm increment to obtain the value of I for each simulated thickness. The value of $\ln(I_0/I)$ is plotted vs. the thickness of the sample. The slope of a linear fit to these data gives μ at the studied photon energy. Other significant shielding parameters can be calculated using μ as explained below.

The mass attenuation coefficient (μ_m) (cm$^2 \cdot$ g^{-1}) of a material is calculated using eq. (2).

$$\mu_m = \mu/\rho, \tag{2}$$

where ρ is the density (g $\cdot$ cm^{-3}) of the absorbing material.

The T is the ratio of the transmitted photon intensity (I) to the incident photon intensity (I_0). Plot of T vs. x can be used to estimate the decrease in the photon intensity with respect to the material thickness. This parameter is calculated as

$$T = I/I_0. \tag{3}$$

The half-value layer (HVL) is the thickness of a material needed to reduce the intensity of the incident radiation by half. Its dependence on μ is defined by eq. (4).

$$\mathrm{HVL} = \ln(2)/\mu. \tag{4}$$

A composite material, like the glass system, is characterised by a number known as effective atomic number (Z_{eff}) which is very helpful to provide conclusive information of a material for nuclear industry, engineering and technological applications. This parameter can be calculated by using the following equation [10]:

$$Z_{eff} = \frac{\sum_i n_i A_i (\mu/\rho)_i}{\sum_i n_i A_i / Z_i (\mu/\rho)_i}, \tag{5}$$

where A_i, n_i and Z_i represent the atomic weight, the number of atoms in the chemical formula and the atomic number of the ith element respectively.

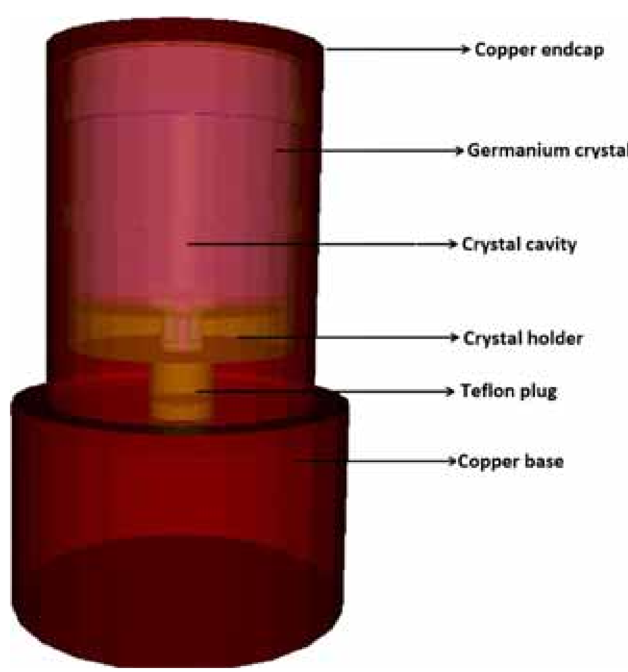

Figure 1. Geant4 model of the HPGe detector used for the determination of μ_m.

2.2 *Monte Carlo simulations*

Photon shielding parameters of the PbBaB glass system were evaluated from the Monte Carlo simulations performed with the Geant4 model of a HPGe ionisation detector and Fluka model of a NaI scintillation detector. Geant4 is a Monte Carlo simulation toolkit used for systems for the high energy, nuclear, accelerator, medical and low energy physics applications. Geant4 is based on the object oriented C++ programming. The Geant4 kernel manages runs, events and tracking of passage of particle through matter [13]. It allows users to simulate all aspects of an experimental set-up such as the geometry of a detector, primary particle generation of events, types of particles and physics processes such as electromagnetic, hadronic and decay physics that manage particle interactions. HPGe detector coded into Geant4 consists of a 2.2 kg germanium crystal installed as an ionisation detector and its complete geometry was coded into Geant4. Figure 1 shows the Geant4 model of the HPGe detector geometry.

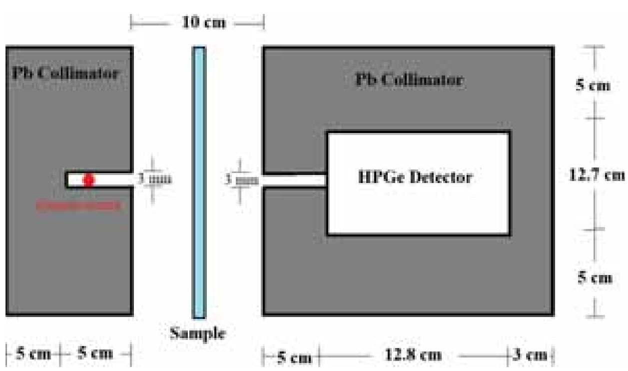

Figure 2. Schematic of the Geant4 set-up.

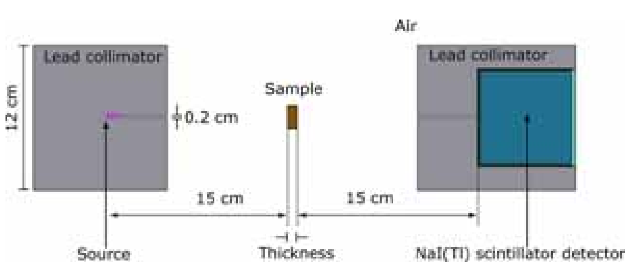

Figure 3. Schematic of the Fluka set-up.

As shown in figure 2, the detector and the γ-ray source are surrounded by a 5 cm thick Pb shield. Stone sample was placed between the source and the detector. Gamma rays emitted by the source are collimated by a Pb collimator, attenuated by the sample and again collimated and detected by the detector. Thanks to the use of narrow beam geometry and Pb collimator, counting of the scattered photons as a part of the transmitted beam is decreased. Therefore, the systematic uncertainties in the measurements are minimised [14].

Similar to Geant4, Fluka simulation toolkit can also be employed to simulate transport and interaction of electromagnetic and hadronic particles within any material [15]. Fluka model of NaI scintillation detector was used to determine the shielding parameters of the selected glass system and a similar simulation set-up was defined to minimise the systematic errors in the Fluka simulations. Figure 3 shows the Fluka set-up used to perform Monte Carlo simulations.

The photon shielding parameters of the selected glasses were determined at the γ-ray energies of 356, 662, 1173 and 1330 keV. Chemical composition, mass fractions and densities of the glass samples were coded into Geant4 and Fluka to define the geometry and the structure of the glass system to perform the Monte Carlo simulations. The values used for the glass samples are shown in table 1.

2.3 *WinXCOM database software*

WinXCom database can also be used to calculate μ_{m} values of any material and this software does not require any experimental set-up [16]. Calculation of the μ_{m} values is based on the mixture rule given by the following equation:

$$(\mu_{\mathrm{m}})_{\mathrm{glass}} = \sum_i w_i (\mu_m)_i, \tag{6}$$

where w_i and $(\mu_m)_i$ are the weight fraction and mass attenuation coefficient of the ith element in the glass structure respectively.

Table 1. Chemical composition parameters of the PbBaB glass system.

	Composition (mol%)				Mass fraction of elements (%)			
Glass sample	PbO	BaO	B_2O_3	Density (g/cm^3)	B	O	Ba	Pb
PbBaB10	10	40	50	4.460	15.529	39.362	35.826	9.283
PbBaB20	20	30	50	4.744	15.529	39.036	26.870	18.566
PbBaB30	30	20	50	5.028	15.529	38.709	17.913	27.850
PbBaB40	40	10	50	5.312	15.529	38.382	8.957	37.133

Table 2. μ_m parameters of the PbBaB glass system obtained from the Monte Carlo simulations, WinXCOM database and experimental values.

Glass sample	356 keV				662 keV				1173 keV				1332 keV			
	Geant4	Fluka	XCOM	Exp.	Geant4	Fluka	XCOM	Exp.	Geant4	Fluka	XCOM	Exp.	Geant4	Fluka	COM	Exp.
PbBaB10	0.129	0.1323	0.1331	0.1327	0.0778	0.0791	0.0795	0.0793	0.0557	0.0558	0.0562	0.0557	0.0531	0.0520	0.0524	0.0517
PbBaB20	0.1479	0.1457	0.1463	0.1462	0.0793	0.0823	0.0862	0.0825	0.0565	0.0656	0.0571	0.0565	0.0528	0.0526	0.0530	0.0524
PbBaB30	0.1520	0.1587	0.1595	0.1572	0.0851	0.0850	0.0856	0.0844	0.0597	0.0574	0.0579	0.0571	0.0566	0.0531	0.0537	0.0529
PbBaB40	0.1654	0.1716	0.1727	0.1711	0.0854	0.0881	0.0886	0.0878	0.0599	0.0582	0.0588	0.0582	0.0563	0.0539	0.0544	0.0539

3. Results and discussion

The Geant4, Fluka and WinXCom results of μ_m values calculated for the PbBaB glass ternary ($x = 10, 20, 30, 40$ mol%) along with the experimental data [17] are given in table 2. The μ_m values were compared to each other in the plots given in figure 4. As can be seen from the comparison plots and from table 2, the computationally obtained μ_m results are in agreement with the experimentally calculated values. This comparison validates the Geant4 and Fluka models of the used detectors to characterise the shielding behaviours of the materials which has not been studied yet. Since high-energy γ-ray photons have more penetration and diffusion ability within the material, μ_m values decrease with the increase of the photon energy and stay almost constant above 1100 keV. This can be clearly seen in figure 4. This trend in μ_m is due to the dominating pair production interaction mechanisms of the photons and at the energy range above 1100 keV and above this energy, interaction mechanism is almost independent of the chemical structures of the studied samples.

Figure 5 shows the dependence of the transmission of γ-ray photons to the thickness of PbBaB10, PbBaB20, PbBaB30 and PbBaB40 glasses at photon energies of 356, 662, 1173 and 1330 keV. Again, due to the high penetration abilities of the high-energy photons, a big difference was observed between 356 and 1330 keV and transmission increases with the increase of photon energy. The transmission values of the PbBaB40 sample for 5 cm glass thickness are 0.0112 and 0.209 at photon energies 356 and 1330 keV respectively. Figure 5 also shows that, among the simulated glasses, the lowest transmissions for all photon energies occur for the PbBaB40 sample and highest transmissions occur for the PbBaB10 sample. This situation can be explained by the higher content of Pb in the PbBaB40 sample compared to the PbBaB10. High atomic number of Pb ($Z = 82$) increases the shielding characteristics of the selected glass system against the γ-ray photons.

The variation of Z_{eff} values as a function of gamma photon energy is shown in figure 6. Z_{eff} of all the glasses with different compositions (mentioned in table 1) are significantly different from each other. With increase of mass fraction of Pb, Z_{eff} of composite glass is found to be increasing which is obvious due to its higher atomic number in comparison with other constituents present. This increase in Z_{eff} with increase of Pb suggests that the shielding ability of glasses get enhanced with the addition of PbO. Among the glasses studied in the present work, PbBaB40 and PbBaB10 possess highest and lowest values of Z_{eff} respectively at photon energies between 356 and 1330 keV. It is observed that Z_{eff} initially decreases sharply until 662

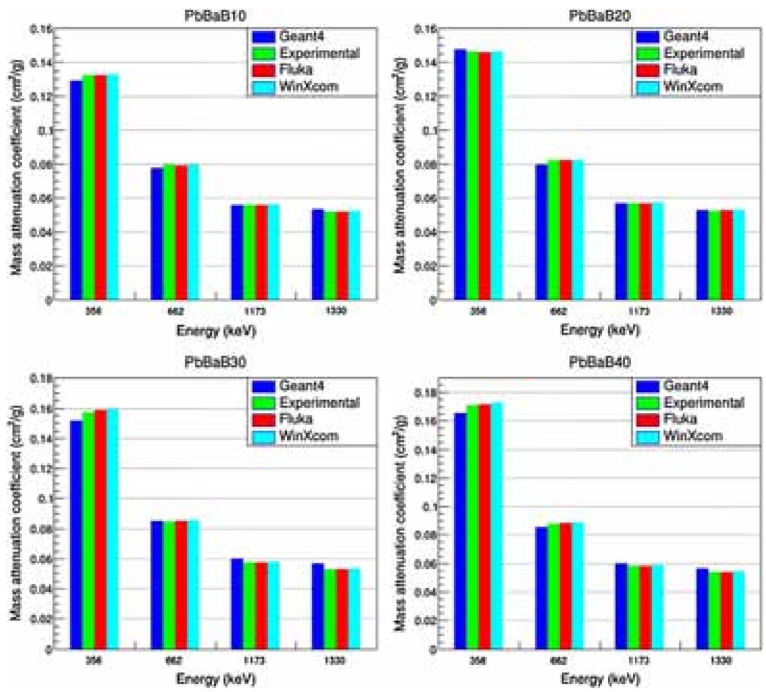

Figure 4. Comparison of the computationally determined μ_m values with the experimental data.

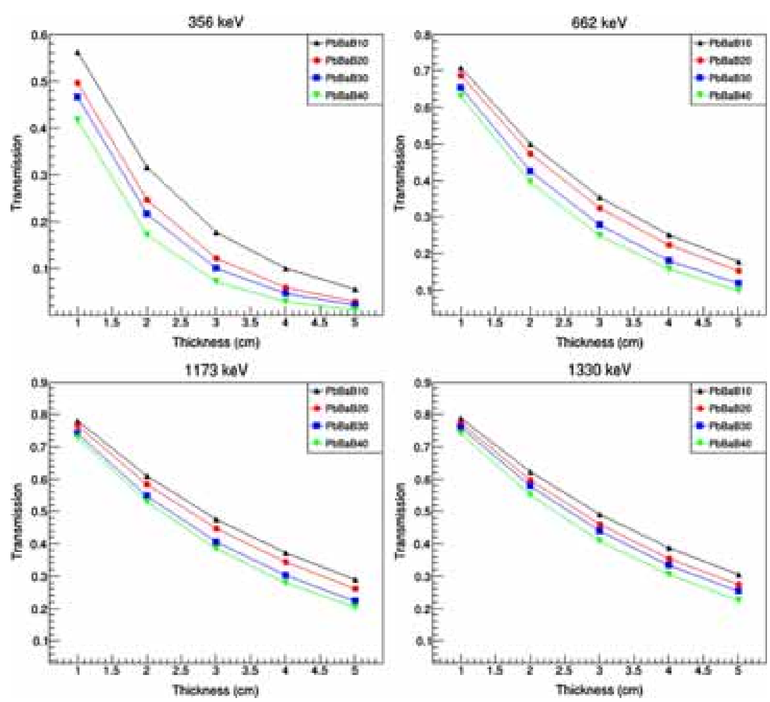

Figure 5. Transmission factor vs. thickness of PbBaB glass system at 356, 662, 1173 and 1330 keV photon energies.

keV. The decrease becomes slower between 662 and 1100 keV and Z_{eff} tends to remain stable on the higher side of γ-ray energy due to the dominance of incoherent (Compton) scattering and pair production processes.

HVL is one of the significant parameters characterising the shielding capability of the PbBaB glass ternary. Lower values of HVL means better shielding performances by using a thin layer of the selected material. In figure 7, HVL values of the PbBaB glass system were

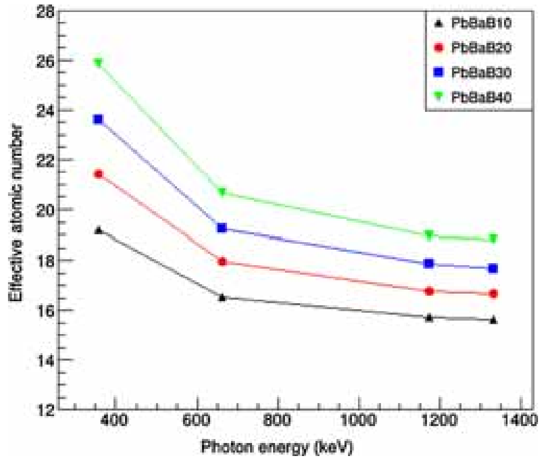

Figure 6. Variation of Z_{eff} with respect to photon energy for the PbBaB glass system.

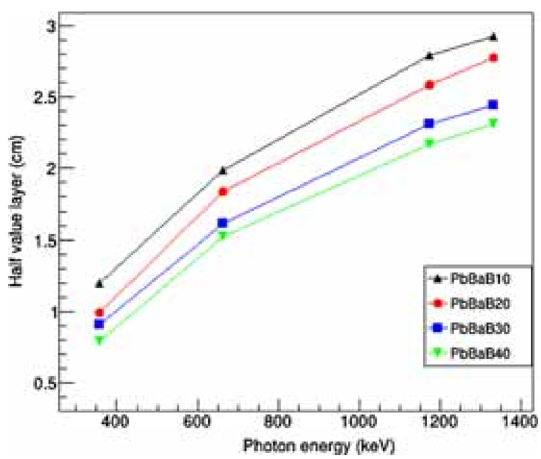

Figure 7. Half value layer of the PbBaB glass system as a function of photon energy.

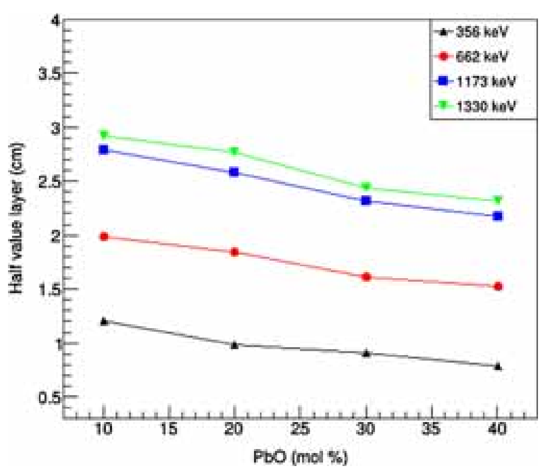

Figure 8. Dependence of HVL on the PbO fraction in the glasses.

plotted with respect to the photon energies. As can be seen in this plot, PbBaB40 has the lowest and PbBaB10 has the highest values of HVL at the given photon energies. Depending on the photon energy, increasing PbO concentration from 10 to 40% causes a decrease of around 34.6 and 20.6% in the HVL at 356 and 1330 keV respectively.

In order to see the dependence of the HVLs on the fraction of PbO, HVL values are plotted vs. 10, 20, 30 and 40% mol of PbO as used in the glass system and the dependencies are shown figure 8. For 10 and 40% mol of PbO, the HVLs change from 1.20 to 0.789 at 356 keV and from 2.92 to 2.31 at 1330 keV. These findings also support that the fraction of PbO in the glass structure significantly affects the shielding abilities of the selected glasses.

4. Conclusion

In this study, μ_{m}, T, HVLs and Z_{eff} of the PbBaB glass system were determined computationally using Geant4, Fluka codes and WinXCOM database software. The obtained μ_{m} were compared with the experimentally calculated values and an agreement was obtained. Thanks to the comparison of the values, the validity of the Geant4 model of HPGe detector and Fluka model of NaI(Tl) detector was proven. μ_{m} has higher values at 356 keV which decreases with increasing γ-ray photon energy and stays almost constant at the energy region above 1100 keV. These trends in mass attenuation are well explained by the various photon interaction processes within the materials. The results of the present study also revealed that the fraction of PbO content in the glass system significantly affects all the shielding parameters and the use of 40% mol of PbO results in a better shielding performance.

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