



Comparison of the Radiation Absorption Properties of PbO doped ZrB₂ Glasses by using GATE-GEANT4 Monte Carlo Code and XCOM Programme

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Abstract:

The aim of this study is to investigate the gamma-ray radiation absorption properties of ZrB₂ (zirconium diboride), which is used in the nuclear industry, space industry, military industry, and especially in the ceramic industry, and determines the effect of PbO additive in the shielding. Also, the Geant4 Application Tomographic Emission (GATE-GEANT4) Monte Carlo computer code tested for its usability in place of the XCOM computer program with an appropriate geometry. Within this scope, the shielding properties of ZrB₂, PbO and 50%ZrB₂.50%PbO glasses at 511, 662, 1173, 1274 and 1332 keV gamma energies were calculated by the GATE-GEANT4 Monte Carlo code and compared with the XCOM computer program. The linear attenuation coefficient and half-value layer were calculated by using the mass attenuation coefficient values obtained with the codes. In line with these results, it is possible to say that 50%PbO additive increases the shielding quality of ZrB₂ glasses. On the other hand, the simulated GATE-GEANT4 Monte Carlo code values were found to be compatible with XCOM..

1. Introduction

In recent years, with technological developments increasing, the use of radiation in many areas such as health, agriculture, and food is increased rapidly. Parallel to this increase, the negative effects of ionizing radiation on health are also increased. Because of the importance of shielding materials in radiation protection, studies on various shielding materials are important in the nuclear field [1]. The choice of gamma radiation protection material is a major component of radiation protection programs. To this end, it is intended to reduce the risk of exposure to ionizing radiation, particularly for workers exposed to radiation. To select the shielding material best suited to a particular source of ionizing radiation, it is necessary to know the basic principles of how gamma rays interact with matter. At the same

time, efforts to identify new shielding materials to replace Pb in terms of cost and ease of use, a heavy metal, have increased [1]. Manufacturing new materials and studying their radiation shielding properties is very expensive in terms of cost and effort. Moreover, studies on radiation are often limited due to economic and ethical rules. For this reason, theoretical methods and statistical approaches developed in today's scientific world play an important role. For this reason, theoretical calculations have come to the fore both in order to examine the shielding properties of more materials and to evaluate the shielding parameters. There are many codes software in which radiation absorption can be displayed by simulation and modelling. With the prepared codes, many types of ionizing radiation like X-rays, γ -rays, electrons, and neutrons can interact with the materials. Many scientific studies examine the radiation absorption properties of

different material mixtures [2, 3]. Boonin et al. [4], synthesized zinc barium telluride glasses and examined their mechanical and structural efficiency as well as their radiation absorption properties at γ -ray energies with Geant4 and WinXCOM software. Cheewasukhanont et al. [5], investigated the radiation shielding parameters of bismuth borosilicate-based glasses with XCOM at 220–662 keV energies and they observed that radiation protection parameters increased with increasing bismuth concentration. Ruengsri et al. [6], showed that the half-value layer (HVL) values of 662 keV of Gd_2O_3 -based glasses with the compositions of $10CaF_2: xGd_2O_3:(90-x)P_2O_5$ ($x = 5, 10, 15, \text{ and } 20$ mole %) can be used in radiation shielding. The mass attenuation coefficients of bismuth borosilicate glasses were obtained by Gerward et al. [7, 8], with the WinXCom program and compared with experimental data. Inoue et al. [9], in their study with ZnO, found a high level of radiation shielding. In another study, the mass attenuation coefficients of lead oxides, bismuth, and barium of silicate glasses was investigated theoretically and experimentally at 662 keV photon energy [10, 11]. Kaewkhao et al. [12], investigated the shielding properties of borate glass containing Bi_2O_3 and BaO at 662 keV and compared it with PbO in the same glass structure. Yasaka et al. [13], investigated the radiation shielding properties and optical properties of zinc bismuth borate (ZBB) glasses. ZBB glass compositions were prepared with the melt quenching technique. Matori et al. [14], and Singh et al. [15], used PbO-based glasses as gamma-ray and X-ray shielding materials and found that they had high absorption properties. Bagheri et al. [16], by using the MCNP code and the XCOM program, investigated the radiation attenuation parameters of barium bismuth borosilicate glasses for gamma-ray energies of 662, 1173, and 1332 keV. In the literature, there are many experimental studies comparing the results obtained in different fields with XCOM data. However, there are limited studies investigating the properties of shielding materials using Geant4-based GATE/GEANT4 simulation. GATE/GEANT4 simulation is a free software program that performs Monte Carlo calculations for use in fields such as radiotherapy, nuclear physics, and radiology. Today, the GATE/GEANT4 simulation has a wide range of uses, from the construction of new medical devices to the development of quality control protocols and medical imaging systems [17, 18]. The XCOM program, on the other hand, calculates the total attenuation coefficient, total attenuation cross-section, and partial cross-section data for various elements, mixtures, and compounds in the photon energy range from 1keV- 100GeV using online

software [8,19]. Physical forms such as photoelectric impact, Compton effect, and pair generation are portrayed in hypothetical calculations. The National Standards Institute (NIST), XCOM database includes radiation attenuation coefficient data of commonly used shielding materials. Zirconium diboride (ZrB_2) is an ultra-high temperature ceramic with a very high melting temperature (3245°C) and a low coefficient of thermal expansion. In addition, it is preferred in the aviation industry and space studies with its high strength, high rigidity, high chemical stability, high thermal shock resistance, low electrical resistance, high voltage capacity, high thermal conductivity, anti-corrosion property and high neutron absorption capacity [20-22]. For these reasons, studies with ZrB_2 have started to increase in recent years [23-29].

This study shows the radiation shielding properties of ZrB_2 , which is a candidate for use in shielding applications and nuclear reactors as a stopper [20]. The study examined and determined alterations in shielding properties through the introduction of a 50% PbO doping. The mass attenuation coefficients (μ_m), linear attenuation coefficients (LAC), and half value layer (HVL) values were calculated using the GATE/GEANT4 Monte Carlo code and XCOM program.

2. Material and Methods

GATE/GEANT4 simulation program is a software in which experimental setup is prepared by making code software in C++ language. First, the element definition of the material to be used as shielding material is made. After the definition is made, the density value and component ratios are entered by creating a compound. When it is desired to create a mixture from different compounds, the density of the compound and the mixing ratios of the components are normalized to one. In the prepared setup, the energy values for the spot welding are manually entered separately and the beam is sent [30]. In the setup prepared to diminish the number of incoming photons, shielding material is put between the source and the detector as given in Fig. 1. In this way, the mass attenuation coefficient of the shielding material is calculated with the prepared setup. In XCOM and GATE/GEANT4 programs, the amount of material can be normalized to 1 and a mixture can be created. Therefore, the relative weights of each compound are given. PbO is the most important material used as a shielding material, and many contributions have been made in the literature to look at the change in absorption properties. The calculations were made by entering the energy values 511, 662, 1173, 1274, and 1332 keV used in the programs. In order to understand the absorption of photons by the matter,

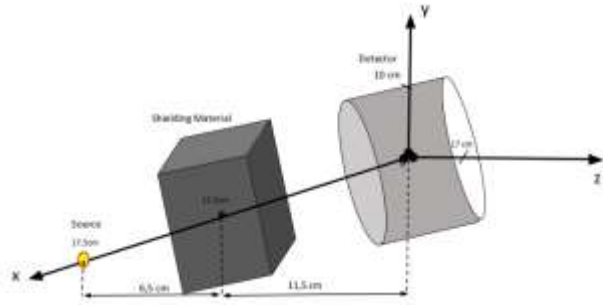


Figure 1. GATE/GEANT4 Experimental setup.

the materials are examined by considering the mass attenuation, linear attenuation, and half-value thickness values. The LAC is a constant for each absorber material. The LAC looks at the reduction in the number of photons per unit distance from the radiation beam passing through the tissue. LAC value increases as the physical density and atomic number of the matter increase.

Theoretical calculations are calculated with the following formulas;

$$\mu_m = (\mu/\rho) \left(\text{cm}^2/\text{g} \right) \quad (1)$$

The mass absorption coefficient (μ/ρ) is independent of chemical and physical states and is a function of wavelength and atomic number.

The amount of photon absorbed by a sample is directly related to the volume of the sample that the photon passes through and the concentration of the sample. This law is the Beer-Lambert law has known and gives the absorption value of the photon [31,32].

$$I = I_0 (e^{-\Gamma x})(e^{-\sigma x})(e^{-\kappa x}) = I_0 e^{-\mu x} \quad (2)$$

In this equation; I is the photon intensity, I_0 is the initial photon intensity, Γ is the photoelectric effect coefficient, σ is the Compton scattering coefficient, κ is the pair production coefficient, and μ is the LAC. The following relations are given for the values of HVL. HVL is the thickness of an absorbent which diminishes the radiation to half its intensity [33]. HVL is determined using the following formulas;

$$HVL = (\ln 2/\mu) \quad (3)$$

3. Results and Discussions

In this study, XCOM software and GATE/GEANT4 simulation program were used together to contribute to the literature, to develop alternative radiation absorbers, and to test the usability of the GATE/GEANT4 Monte Carlo code for radiation absorption. The LAC and the HVL of the ZrB_2 , PbO , and PbO -doped ZrB_2 samples have been calculated.

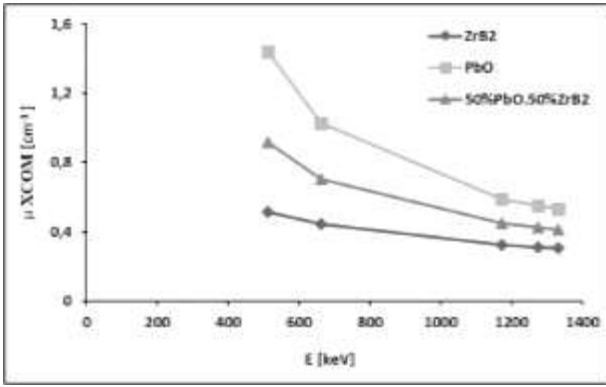
Obtained values are given comparatively. In addition, the LAC (μ) was evaluated using the XCOM program to confirm the GATE/GEANT4 Monte Carlo code (Table 1 and Fig. 2-a and Figure 2-b). The difference percent (Diff. %) between the two simulations was calculated using Eq. (4) and shown in Table 1 [34].

$$\text{Diff} (\%) = \frac{\mu_{\text{xcom}} - \mu_{\text{gate}}}{\mu_{\text{xcom}}} \times 100\% \quad (4)$$

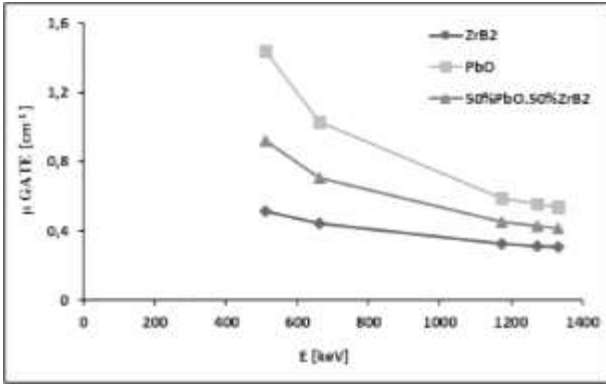
Table I: Calculated values for LAC

ZrB₂			
Energy (keV)	XCOM	GATE	%Diff.
511	0.514	0.517	-0.446
662	0.443	0.446	-0.755
1173	0.325	0.328	-0.802
1274	0.311	0.314	-0.763
1332	0.304	0.307	-0.710
PbO			
Energy (keV)	XCOM	GATE	%Diff.
511	1.441	1.440	0.044
662	1.027	1.030	-0.268
1173	0.587	0.591	-0.718
1274	0.551	0.555	-0.695
1332	0.534	0.538	-0.642
50%ZrB₂.50%PbO			
Energy (keV)	XCOM	GATE	%Diff.
511	0.920	0.921	-0.132
662	0.704	0.708	-0.476
1173	0.449	0.452	-0.766
1274	0.425	0.428	-0.727
1332	0.414	0.417	-0.674

The Diff. % values varied from 0.044% to -0.802% for all energy values, respectively. These values indicate that the simulated GATE/GEANT4 values agree with the computed XCOM values. Figure 2-a and Figure 2-b appears that the XCOM (a) and GATE/GEANT4 (b) values for LAC as a function of the photon energy graph for ZrB_2 , PbO , and 50% ZrB_2 .50% PbO . It is seen that the addition of PbO provides more than 55% increase in the LAC values of ZrB_2 . The calculated LAC values using the XCOM at the incident energy range (0.001 MeV to 10^5 MeV) are shown in Fig.3(a,b,c). In the energy values calculated within the study, the attenuation coefficient of uptake appears to diminish as the energy increases. The simulated GATE/GEANT4 values are in agreement with the XCOM and this shows the accuracy of the simulated values. The calculated HVL values using GATE/GEANT4 and XCOM are shown in Fig. 4-a,b,c.

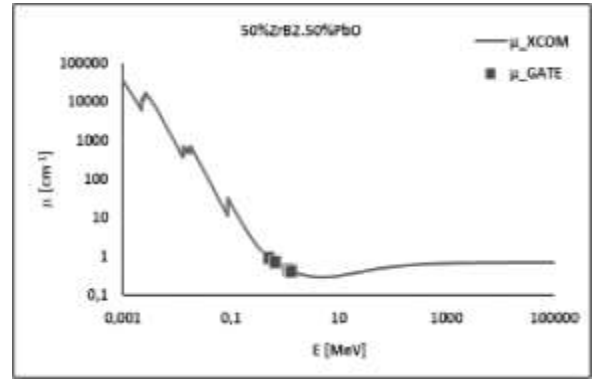


(a)



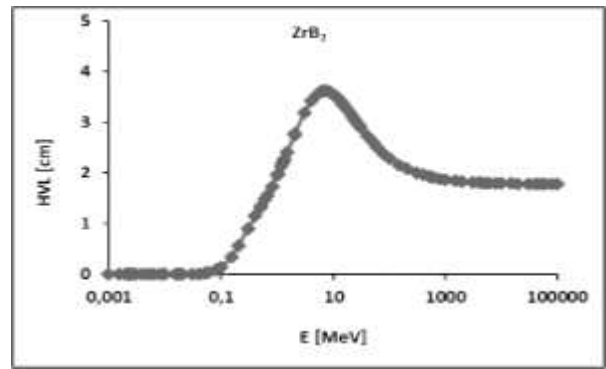
(b)

Figure 2. Calculated XCOM (a) and GATE/GEANT4(b) values for LAC as a function of the photon energy graph for ZrB₂, PbO, and 50%ZrB₂.50%PbO.

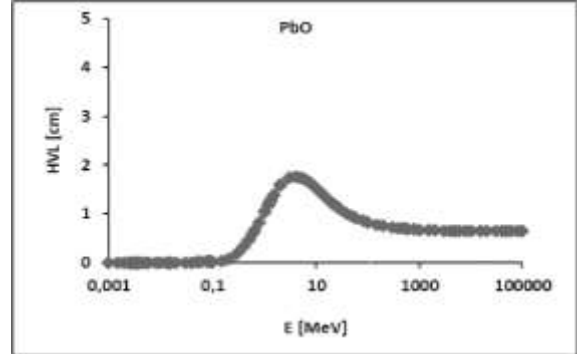


(c)

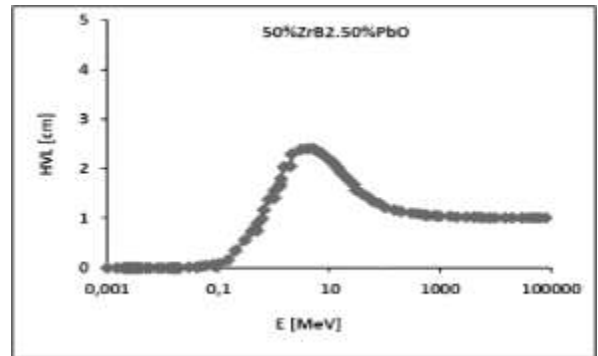
Figure 3. XCOM and GATE/GEANT4 values for LAC as a function of photon energy (0.001 MeV to 10⁵ MeV) for ZrB₂ (a), PbO(b) and 50%ZrB₂.50%PbO (c).



(a)



(b)



(c)

Figure 4. HVL as a function of photon energy (0.001 MeV to 10⁵ MeV) for ZrB₂ (a), PbO (b) and 50%ZrB₂.50%PbO (c).

Figure 4 clearly appears that the concentration of PbO included to ZrB₂ causes an diminish in HVL values of 50%ZrB₂.50%PbO.

4. Conclusions

The purpose of this study is to study the absorption properties of ZrB₂ gamma rays, which has just begun to be used in many areas, particularly in the ceramic industry.

In XCOM and GATE/GEANT4, LAC and HVL and values, which are radiation absorption coefficients, were calculated by defining the density values and chemical formulas separately for the mixture and single chemicals.

The data from the GATE/GEANT4 simulation were observed to be consistent with the XCOM data in the appropriate geometry, and moreover determined to added by the 50%PbO provides more than 55% increase in the LAC values of ZrB₂.

Author Statements:

- **Ethical approval:** The conducted research is not related to either human or animal use.
- **Conflict of interest:** The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper
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- **Data availability statement:** The data that support the findings of this study are available on request from the corresponding author. The data are not publicly available due to privacy or ethical restrictions.

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