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A Comprehensive Study on the Effect of $BaSO_4$ on Gamma-Ray Shielding Properties of B_2O_3-CaO-Na_2O-SiO_2 Glass System, a Comparative Evaluation Using Phy-X / PSD and XMuDat Program

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***Abstract*— The mass attenuation coefficient (μ_m), linear attenuation coefficients (μ), half value layer (HVL), mean free path (MFP), total atomic cross section (ACS), total electronic cross section (ECS), and effective atomic number (Z_{eff}) are determined in this research because they are the most important radiation attenuation coefficients and play a significant role in the fields of radiography, radiotherapy, and prevention of ionizing radiation.**

Gamma ray shielding properties of silicate glasses ($10B_2O_3$-10CaO-$20Na_2O$-(60- x) SiO_2- x $BaSO_4$) with ($0 \le x \le 40$ wt%) have been achieved. The attenuation coefficients for gamma rays were calculated theoretically with the help of the Phy-x program, and then these values were compared with the results obtained using the XMuDat program. Variations of shielding parameters are discussed for the effect of $BaSO_4$ addition into the glasses and photon energy of range from (0.003-3) MeV including the radioactive sources ^{22}Na, ^{60}Co, ^{131}I, and ^{137}Cs.

Glass with the highest doping concentration achieved the optimum values for μ_m, μ, and Z_{eff}. The lowest values of MFP and HVL for the glasses were observed for intermediate energies of gamma photons.

The computed values of various attenuation coefficients for gamma rays like μ_m, μ, HVL MFP, ACS, ECS, and Z_{eff} derived from the XMuDat program were in good agreement with the theoretical values resultant using the Phy-X program. The proposed glass system of the form ($10B_2O_3$-10CaO-$20Na_2O$-$20SiO_2$-$40BaSO_4$) may be useful for many shielding applications.

***Keywords*— Silicate glass, $BaSO_4$, Gamma photons energy, Attenuation coefficient, Effective atomic number.**

I. INTRODUCTION

Radioactive isotopes such as ^{99m}Tc (Technetium-99 m), ^{60}Co (Cobalt-60) are used in radiological diagnosis (gamma camera and positron imaging) and radiotherapy, such as ^{131}I (Iodine -131). Radioisotopes usually emit ionizing radiation (alpha and beta particles) or electromagnetic radiation (x-rays and gamma rays). The ability of gamma rays to penetrate is high, so they pass long distances in materials, for this reason, gamma rays are considered the most dangerous type of ionizing radiation. Radiation exposure can cause cancer and death by destructing living cells and tissues. Because of their high energy and penetrability, attenuating gamma rays is difficult and requires an adequate radiation shielding material to protect working personnel [1-3]. The shielding materials must have good radiation attenuation, high density, and low toxicity in manufacturing [4-5].

Previously, materials that are not visible to light, such as polymers, cement, and ceramics, were used to protect against gamma radiation [6-8].

Currently, efforts have been made to manufacture and develop types of glass for radiation protection, as this glass is used in the windows and doors of radiation therapy units and medical diagnostic laboratories (X-ray and CT)[9-10].

Recently, there has been a trend towards manufacturing types of glass, such as silicate glass, as materials for radiation protection from ionizing radiation [11].

Barium is a good absorbent of gamma radiation due to its high density. Using barite ($BaSO_4$) is a good choice to protect against radiation. Barite is one of the most economically environment-friendly shielding materials [12]

The most important radiation attenuation coefficients used in radiation protection are: the linear attenuation coefficient (μ), mass attenuation coefficient (μ_m), half value layer (HVL), mean free path (MFP), effective atomic number (Z_{eff})[5,13-15].

Several programs are developed to help investigate different glasses and calculate the attenuation coefficients of gamma ray such as XCOM [16], WinXCom [17], Phy-X/PSD [18], XMuDat [19], Py-MLBUF [20].

B.Al-Bahiri et al. [21] calculated the attenuation coefficient of NiO-doped B_2O_3–$BaCO_3$–Li_2O_3 glass using

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the WinXCOM program . Chanthima et al [22] determined the attenuation coefficients of $BaSO_4$ and PbO doped cement from gamma rays.

The present work aims to study the effectiveness of $BaSO_4$ on radiation attenuation parameters of silicate glasses of composition $10B_2O_3$-10CaO-$20Na_2O$-(60-x)SiO_2- x $BaSO_4$ (x = 0, 10, 20, 30and 40wt%). The radiation attenuation parameters of silicate glasses were theoretically determined by using Phy-X/PSD software [18]. We made a comparison between the results obtained with the Phy-x and XMuDat programs [19].

II. COMPUTATIONAL METHODS

In this work, we calculated the radiation attenuation coefficient of GS (B_2O_3-CaO-Na_2O-SiO_2) doped with $BaSO_4$ in the photon energy range of (0.003-3) MeV theoretically by using the Phy-X and XMuDat programs

A.Phy-X/PSD software

Phy-X/PSD software can calculate shielding parameters for different materials in the continuous energy range and selected energies [18]. Radiation attenuation parameters such as mass attenuation coefficient (μ_m), linear attenuation coefficient (μ), half value layer (HVL), mean free path (MFP), and effective atomic number (Z_{eff}), are calculated in a certain or continuous energy region. Phy-X / PSD is free to use at https://phy-x.net/PSD.

B. XMuDat software

The XMuDat software can calculate partial and total mass attenuation coefficients for photon interactions with materials (elements, mixtures, and compounds) within the energy range (0.001-50) MeV [19].

C. Determination of gamma-ray attenuation coefficient

The mass attenuation coefficient (μ_m) is equivalent to the linear attenuation coefficient divided by the density of the absorber. The next relation is used for the determination of this parameter [23].

$$\mu_m\left(\frac{cm^2}{gr}\right)=\frac{\mu}{\rho} \qquad (1)$$

For composite materials (e.g, glass), the (μ_m) is given by the following relation [24,25]

$$\mu_m=\sum_i w_i(\mu_m)_i \qquad (2)$$

where $(\mu_m)_i$ is the mass attenuation coefficient of the ith constituent element and w_i is the weight fraction of the ith constituent element in the glass sample.

The half-value layer (HVL) is the thickness, at which the transmitted intensity is 50% of the initial intensity [26]. (HVL) of the glasses can be calculated from the following formula [27].

$$HVL=\frac{\ln(2)}{\mu}=\frac{0.693}{\mu} \qquad (3)$$

where μ is the glass linear attenuation coefficient.

The mean free path can be calculated from the information of the linear attenuation coefficient according to the following relation [13].

$$MFP=\frac{1}{\mu} \qquad (4)$$

The total atomic cross section (ACS), the total electronic cross section (ECS), and the effective atomic number (Z_{eff}) for any sample can be calculated using the following expression [28,29].

$$ACS=\sum_i f_i A_i\,(\mu_m)_i \qquad (5)$$

$$ECS=\sum_i \frac{f_i A_i}{Z_i}(\mu_m)_i \qquad (6)$$

$$Z_{eff}=\frac{ACS}{ECS}=\frac{\sum_i f_i A_i(\mu_m)_i}{\sum_i \frac{f_i A_i}{Z_i}(\mu_m)_i} \qquad (7)$$

where f_i, A_i, and Z_i refer to the fractional abundance, atomic weight, and atomic number of the ith constituent element respectively.

III. RESULTS AND DISCUSSION

Gamma photon interaction parameters like μ_m, μ, HVL MFP, and Z_{eff} of silicate glass system with a nominal composition ($10B_2O_3$-10CaO-$20Na_2O$-(60- x) SiO_2- $x$$BaSO_4$ (x = 0, 10, 20, 30 and 40 wt%)) have been investigated. Table.1 displays the densities, and weight fractions of elements in each glass sample obtained using the Phy-X and XMuDat programs.

Table 1: Weight fractions of elements and densities of $BaSO_4$-doped silicate glasses

	Weight Fraction of Elements (Wt %)							
sample ID	Boron (B)	Barium (Ba)	Calcium (Ca)	Oxygen (O)	Sodium (Na)	Sulfur (S)	Silicon (Si)	Density (g/cm^3)
GS	0.0310	0.0	0.0715	0.4686	0.1484	0.0	0.2805	2.31
GS+10 $BaSO_4$	0.0310	0.0588	0.0715	0.4428	0.1484	0.0137	0.2337	2.43
GS+20 $BaSO_4$	0.0310	0.1177	0.0715	0.4169	0.1484	0.0275	0.1870	2.56
GS+30 $BaSO_4$	0.0310	0.1765	0.0715	0.3911	0.1484	0.0412	0.1403	2.71
GS+40 $BaSO_4$	0.0310	0.2354	0.0715	0.3653	0.1484	0.0550	0.0935	2.87

The mass attenuation coefficient (μ_m) of glass samples was theoretically calculated by using the Phy-X/PSD program for the photons with energies ranging from 3 KeV to 3 MeV and selected energies radioactive sources ^{22}Na(0.511, 1.28)MeV,^{60}Co(0.347, 0.826, 1.17, 1.33, 2.5) MeV, ^{131}I(0.365, 0.723, 0.637) MeV, and ^{137}Cs (0.284, 0.662)MeV [18]. A comparative study was also developed between the results of the above program and the results of the XMuDat program which are shown in figure.1.

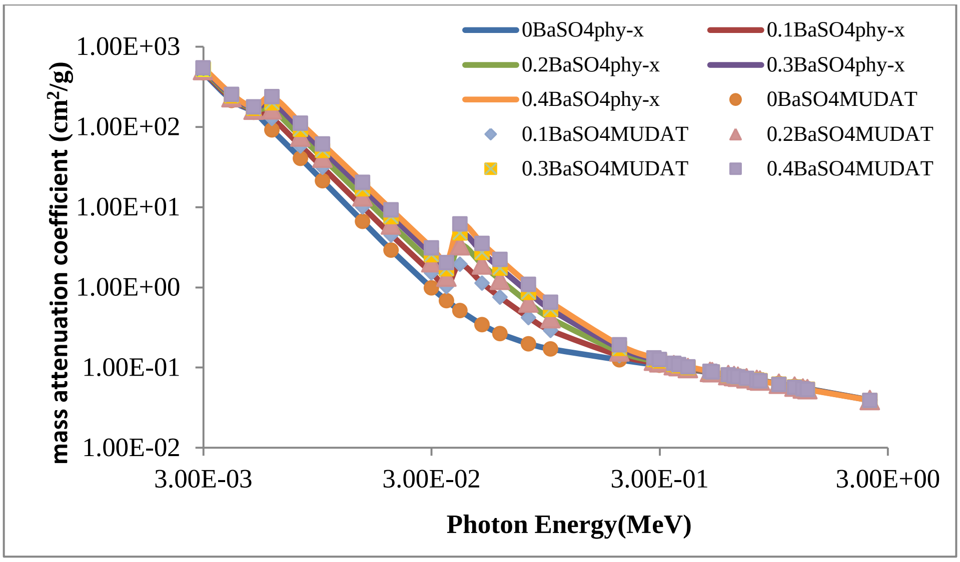

Fig. 1: Comparison of the phy-X and XMuDat calculated values of linear attenuation coefficient (μ_m) versus photon energy for glass samples.

Fig.1 demonstrates the variation of μ_m values with photon energy for the glasses $10B_2O_3$-10CaO-$20Na_2O$-(60-x) SiO_2- $x BaSO_4$ with ($0 \leq x \leq 40$ wt %). The computed values of μ_m, derived from XMuDat programs were in good agreement with the theoretical values acquired using the Phy-X program. μ_m of all the glass samples has the same photon energy dependence, and it significantly increases as $BaSO_4$ content increases in the glass sample.

We notice from Figure1 that in the region of low energies at 0.003MeV, the proposed glass has the maximum values of the mass attenuation coefficient, and after that, there is a rapid decrease in the values of the coefficient with increasing gamma photon energy. After that above 0.3MeV, the μ_m values have a very weak dependence on the gamma photon energy. This can be explained as follows: In the low-energy region, the photoelectric effect dominates, as the absorption coefficient changes with $1/E^3$, and then a sudden change occurs in the curve of μ_m at (0.037 and 0.006) MeV due to the K and L absorption edge of Ba element [22]. In the region of medium energies (0.1-1) MeV, Compton scattering dominates, which is inversely proportional to the energy E, while at energies higher than 1MeV, the pair production effect dominates, which is inversely proportional to the logE[30].

Gamma photons of different energies ranging (0.284–2.51) MeV were obtained from the radioactive sources ^{22}Na, ^{60}Co, ^{131}I, and ^{137}Cs. The values of μ, HVL, and MFP of the glass samples were obtained using the XMuDat program and compared theoretically with the acquired using the Phy-X program.

The total linear attenuation coefficient (μ) can be calculated by multiplying the mass attenuation coefficients by the density of compounds, as illustrated in Equation 1 and the results are shown in Table.2.

Table 2:The linear attenuation coefficient (μ) utilizing phy-X and XMuDat for glass samples, in different photon energies

E (MeV)	$0BaSO_4$ phy-x	$0.1BaSO_4$ phy-x	$0.2BaSO_4$ phy-x	$0.3BaSO_4$ phy-x	$0.4BaSO_4$ phy-x	$0BaSO_4$ MUDAT	$0.1BaSO_4$ MUDAT	$0.2BaSO_4$ MUDAT	$0.3BaSO_4$ MUDAT	$0.4BaSO_4$ MUDAT
0.284	0.252	0.279	0.309	0.343	0.379	0.252	0.279	0.310	0.341	0.379
0.347	0.233	0.252	0.273	0.297	0.324	0.231	0.253	0.274	0.298	0.324
0.365	0.228	0.246	0.266	0.288	0.313	0.228	0.245	0.266	0.287	0.313
0.511	0.198	0.210	0.223	0.238	0.254	0.198	0.210	0.223	0.237	0.253
0.637	0.180	0.190	0.200	0.212	0.225	0.180	0.189	0.200	0.212	0.224
0.662	0.177	0.186	0.196	0.208	0.220	0.177	0.186	0.196	0.208	0.220
0.723	0.170	0.179	0.188	0.199	0.210	0.170	0.178	0.188	0.198	0.210
0.826	0.160	0.168	0.176	0.186	0.196	0.160	0.167	0.176	0.185	0.196
1.170	0.135	0.141	0.147	0.155	0.163	0.134	0.140	0.147	0.154	0.162
1.280	0.129	0.135	0.141	0.148	0.156	0.128	0.134	0.140	0.147	0.155
1.330	0.126	0.132	0.138	0.145	0.153	0.126	0.131	0.138	0.145	0.152
2.510	0.0912	0.0957	0.101	0.106	0.112	0.0908	0.0953	0.100	0.106	0.112

Fig.2 illustrates the gamma photons energy-dependent variation of linear attenuation coefficients (μ) of the glasses obtained by the two programs XMuDat and Phy-X.

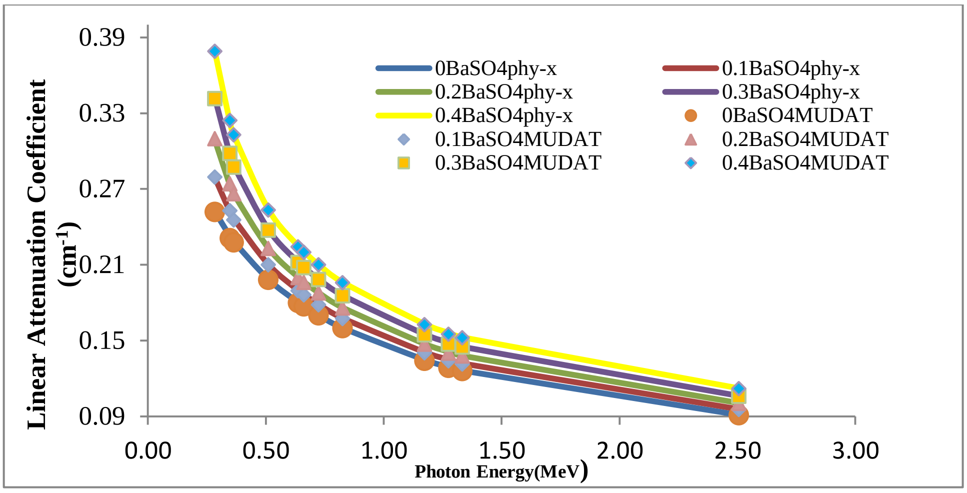

Fig. 2 :Comparison of the phy-X and XMuDat calculated values of linear attenuation coefficient (µ) versus photon energy for glass samples.

The HVL and MFP values were calculated from equations (3,4) and the results were listed in the tables3and 4, respectively.

Table 3: Half value layer (HVL) utilizing phy-X and XMuDat for samples, in different photon energies.

E (MeV)	$0BaSO_4$ phy-x	$0.1BaSO_4$ phy-x	$0.2BaSO_4$ phy-x	$0.3BaSO_4$ phy-x	$0.4BaSO_4$ phy-x	$0BaSO_4$ MUDAT	$0.1BaSO_4$ MUDAT	$0.2BaSO_4$ MUDAT	$0.3BaSO_4$ MUDAT	$0.4BaSO_4$ MUDAT
0.284	2.75	2.48	2.24	2.02	1.83	2.75	2.48	2.24	2.03	1.83
0.347	2.98	2.75	2.54	2.33	2.14	3.00	2.74	2.53	2.32	2.14
0.365	3.04	2.81	2.61	2.40	2.22	3.05	2.82	2.60	2.41	2.21
0.511	3.49	3.30	3.11	2.91	2.73	3.50	3.30	3.11	2.92	2.74
0.637	3.85	3.65	3.46	3.27	3.08	3.86	3.66	3.47	3.27	2.86
0.662	3.91	3.72	3.53	3.33	3.15	3.92	3.72	3.53	3.34	3.15
0.723	4.07	3.88	3.69	3.49	3.30	4.08	3.89	3.69	3.49	3.30
0.826	4.33	4.13	3.94	3.73	3.53	4.34	4.14	3.95	3.74	3.53
1.170	5.14	4.92	4.70	4.47	4.25	5.17	4.94	4.72	4.49	4.28
1.280	5.37	5.14	4.91	4.67	4.44	5.41	5.18	4.95	4.71	4.47
1.330	5.49	5.26	5.02	4.78	4.54	5.50	5.27	5.03	4.79	4.56
2.510	7.60	7.24	6.89	6.53	6.18	7.63	7.28	6.92	6.56	6.18

Table 4: Mean free path (MFP) utilizing phy-X and XMuDat for glass samples in different photon energies.

E (MeV)	$0BaSO_4$ phy-x	$0.1BaSO_4$ phy-x	$0.2BaSO_4$ phy-x	$0.3BaSO_4$ phy-x	$0.4BaSO_4$ phy-x	$0BaSO_4$ MUDAT	$0.1BaSO_4$ MUDAT	$0.2BaSO_4$ MUDAT	$0.3BaSO_4$ MUDAT	$0.4BaSO_4$ MUDAT
0.284	3.97	3.58	3.24	2.92	2.64	3.97	3.58	3.23	2.93	2.64
0.347	4.30	3.97	3.66	3.36	3.09	4.33	3.96	3.65	3.35	3.09
0.365	4.38	4.06	3.76	3.47	3.20	4.39	4.07	3.76	3.48	3.19
0.511	5.04	4.76	4.48	4.20	3.94	5.05	4.76	4.49	4.21	3.95
0.637	5.55	5.27	5.00	4.72	4.45	5.56	5.28	5.01	4.72	4.46
0.662	5.65	5.37	5.09	4.81	4.54	5.65	5.37	5.10	4.82	4.55
0.723	5.88	5.60	5.32	5.03	4.76	5.89	5.61	5.33	5.04	4.76
0.826	6.25	5.96	5.68	5.38	5.10	6.26	5.97	5.69	5.39	5.10
1.170	7.42	7.10	6.79	6.45	6.13	7.46	7.13	6.81	6.47	6.17
1.280	7.75	7.41	7.08	6.74	6.40	7.80	7.47	7.14	6.80	6.45
1.330	7.92	7.58	7.25	6.89	6.55	7.94	7.61	7.26	6.91	6.58
2.510	10.97	10.45	9.95	9.42	8.91	11.02	10.50	9.99	9.46	8.82

The tables 3 and 4 display the changes in the HVL and MFP values of the proposed glasses with gamma photon energy. Showed good agreement between calculated and theoretical results. The sample of glass doped ($0.4BaSO_4$) represents the best shield system. Gamma rays lose a large portion of their energy when they interact with glass samples of large density.

The total linear attenuation coefficients (μ) for the Concrete Barite, Concrete Ordinary, and silicate glasses doped $BaSO_4$(x = 0, 10, 20, 30 and 40wt%)) were calculated by the programs phy-X and XMuDat for photon gamma of the energy range (0.284–2.51) MeV of gamma rays radioactive sources ^{22}Na, ^{60}Co, ^{131}I, and ^{137}Cs, and shown in Figure 3.

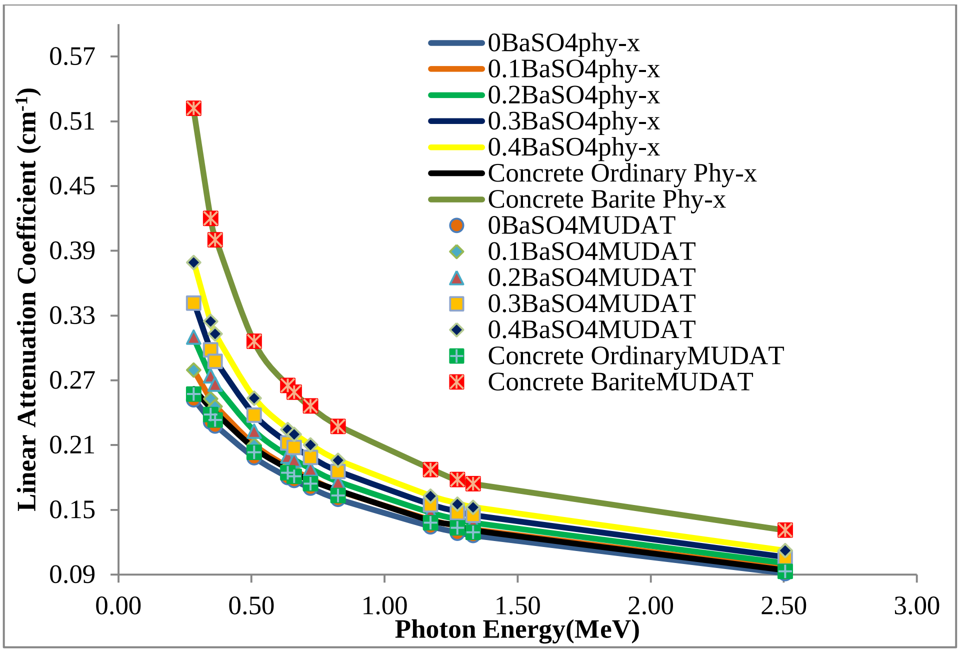

Fig.3: Comparison of the phy-X and XMuDat calculated values of linear attenuation coefficient (μ) versus photon energy for glass samples, Concrete ordinary, and Concrete Barite.

Fig.3 shows the relationship between the μ values and gamma photon energy of the energy range (0.284–2.51) MeV for glass samples, Concrete ordinary, and Concrete Barite, gradually decreasing with increasing gamma energy up to 2MeV, then its values decrease slightly to energies greater than that value.

The behavior of the total linear attenuation coefficients μ in the gamma ray shielding of the glass composites is similar to that of the concrete ordinary, Concrete Barite, but with lower values for concrete ordinary. Concrete Barite has the highest linear attenuation coefficient values due to its high density ($3.35g/cm^3$).

The values of μ increase with the increase in $BaSO_4$ concentration added to the silicate glass system, the highest concentration of glass ($0.4BaSO_4$) represents the best shield over all the photon energy range. Fig.3 shows a good agreement between the calculated and theoretical results of the linear attenuation coefficient values, for all studied shielding samples.

ACS and ECS of the glasses were calculated from equations (5,6). The radiation shielding parameters of the silicate glass containing $BaSO_4$ was theoretically calculated by using Phy-X/PSD program and then compared with the results obtained using the XMuDat program for gamma photon energy (0.003-3)MeV and selected energies radioactive sources ^{22}Na, ^{60}Co, ^{131}I, and ^{137}Cs. The figures (4,5) show the variations of the calculated values versus photon energies.

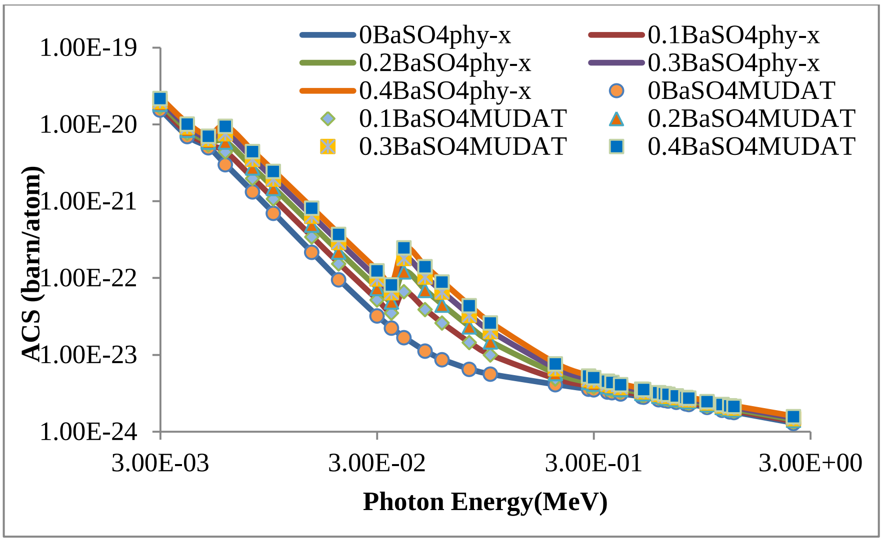

Fig. 4:Comparison of the phy-X and XMuDat calculated values of ACS versus photon energy for glass samples.

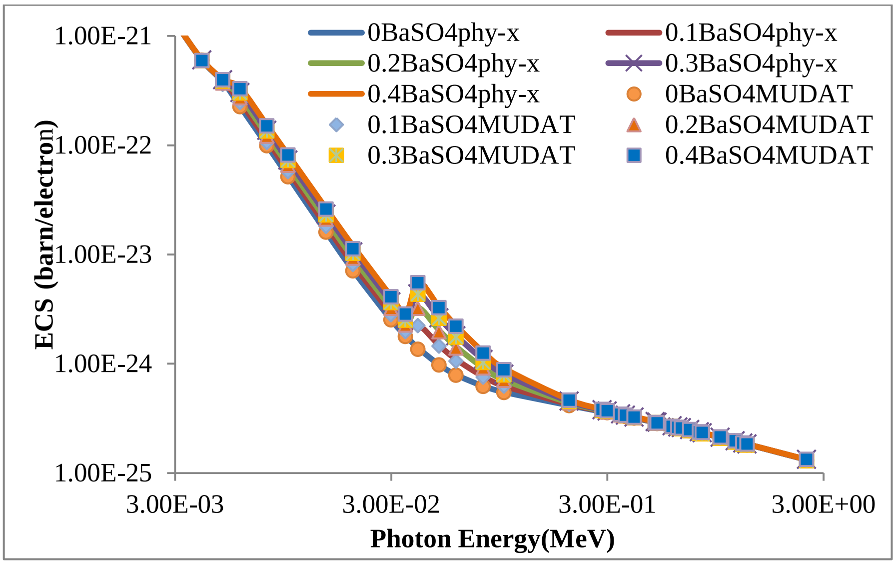

Fig5: Comparison of the phy-X and XMuDat calculated values of ECS versus photon energy for glass samples.

Figs (4 and 5) show the changes of ACS and ECS with gamma photon energy, which show that the values of ACS and ECS increased with increasing $BaSO_4$ concentration in the glass while decreasing with increasing gamma photon energy.

It is also clear that the glass Sample (GS+40%$BaSO_4$) has the highest atomic cross section (ACS) and the total electronic cross section (ECS). This is due to the high values of mass attenuation coefficients of the elements. (GS+40%$BaSO_4$) contains the highest percentage of barium and is among high-density shielding materials.

Z_{eff} the effective atomic number values of (B_2O_3-CaO-Na_2O-SiO_2-$BaSO_4$) were calculated from equation 7 and plotted in figure.6. It shows the changes in the effective atomic number of the proposed glass with the gamma photon energy (0.003-3)MeV obtained with the two programs XMuDat and Phy-X. We note good agreement between the values.

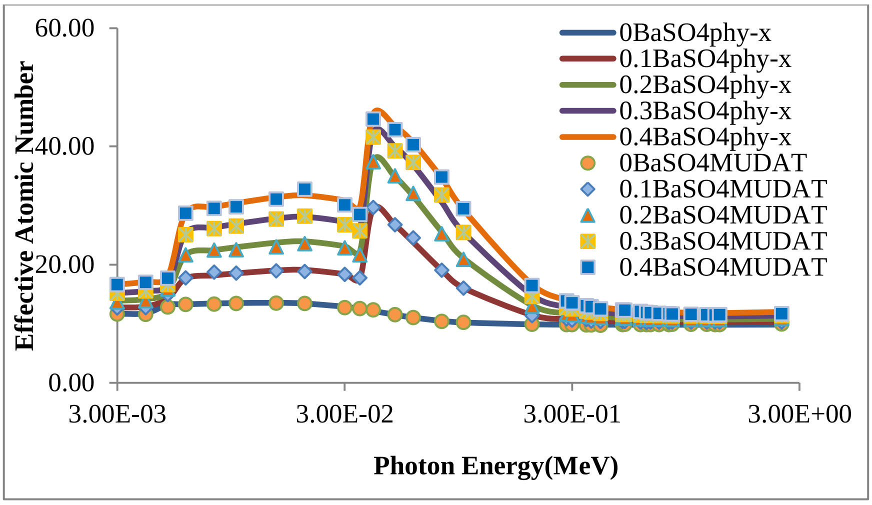

Fig.6: Comparison of the phy-X and XMuDat calculated values of effective atomic number versus photon energy for glass samples.

We note that the Z_{eff} values increase in the low-energy region (0.003-0.03) MeV, with two peaks appearing at gamma photon energies of 0.037 and 0.006MeV due to the K and L-absorption edge of Ba element [22]. Z_{eff} decreases sharply in the energy region (0.04-0.3) MeV. At energy above 0.3MeV, the Z_{eff} values become almost constant. This can be explained by the relation of the partial photon processes with the atomic number Z of the glass constituent elements, where at low energies the photoelectric effect, which is proportional to Z^{4-5}, dominates, while at medium energies the Compton effect, which is proportional to Z^2, dominates[31–33].

From Figure 6 we found Z_{eff} values are high for silicate glass containing ($0.4BaSO_4$) in all energies. Due to the higher Z_{eff} value, it can be said that silicate glass containing ($0.4BaSO_4$) has the highest shielding potential among others.

IV.CONCLUSIONS

In this work, we determined the gamma ray shielding properties of glass ($10B_2O_3$-10CaO-$20Na_2O$-(60- x) SiO_2- x $BaSO_4$) with ($0 \leq x \leq 40$ wt%).

The μ_m, ACS, ECS, Z_{eff} parameters were calculated in the range of (0.003-3) MeV including the energies of radioactive sources ^{22}Na, ^{60}Co, ^{131}I, and ^{137}Cs. The μ, HVL, MFP values of the proposed glasses were calculated in the range of gamma photon energies (0.284–2.51) MeV. The attenuation coefficients of the silicate glass calculated theoretically using the Phy-x program were compared with those resulting from using the XMuDat program, and good agreement was observed between them.

The results of calculating the linear attenuation coefficients (μ), the half value layer (HVL), and the mean free path (MFP) of the proposed glass system at the photon gamma energy with the energy rang (0.284–2.51) MeV showed the decrease of the linear attenuation coefficients μ values and the increase of the values of other attenuation coefficients within the photons gamma energy. The results also showed that the linear attenuation coefficients μ increase exponentially by increasing the concentration of $BaSO_4$ in the proposed glass, while the values of HVL and MFP decrease linearly with increasing concentration of $BaSO_4$.

By comparing the theoretical results of the linear attenuation coefficient of gamma photons for Concrete Ordinary, Concrete Barite, and silicate glass doped $BaSO_4$ with the results obtained using a program, we notice that the behavior of the total linear attenuation coefficients μ in the gamma ray shielding of the glass composites is similar to that of the concrete ordinary, Concrete Barite, but with lower values for concrete ordinary. While Concrete Barite has the highest linear attenuation coefficient values due to its high density.

We concluded from the total atomic cross-section (ACS) and the total electronic cross-section (ECS) values that the best glass sample for shielding from gamma rays is the one containing ($0.4BaSO_4$),

The effective atomic number (Z_{eff}) increases with sample density. The sample content (0.4 $BaSO_4$) with the highest density (2.87 g/cm^3) has the highest shielding potential from gamma rays of all the shielding glass samples.

We found good agreement between the calculated effective atomic number (Z_{eff}) values and theoretical results, and that the highest values of the effective atomic number were achieved in the energy region (0.006–0.1)MeV.

From the previous results, we concluded that a glass sample of the form ($10B_2O_3$-10CaO-$20Na_2O$-$20SiO_2$-$40BaSO_4$) has the best shielding properties against gamma radiation within the energy between (0.003-3) MeV, therefore, it could be a potential candidate for gamma radiation shielding applications.

The mass attenuation coefficient, linear attenuation coefficient, and the effective atomic number for the glass Sample (GS+40%$BaSO_4$) are higher than the other proposed glass samples. The half-value layer and mean free path are lower for (GS+40%$BaSO_4$) than the other proposed glass samples. Among the studied glass Samples (GS+40%BaSO4) is the best material for gamma ray shielding.

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CONFLICT OF INTEREST

Authors declare that they have no conflict of interest.

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