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Research article

The Calculation of Photon Interactions in $Gd_2YAl_2Ga_3O_{12}$ compound by the Phy-X Software Compared with WinXCom Program

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Abstract

The photon interactions in $Gd_2YAl_2Ga_3O_{12}$ compound were studied in this work. The interaction parameters, such as total mass attenuation coefficient (μ_m), effective atomic number (Z_{eff}), effective electron density (N_{eff}), mean free path (*MFP*), half-value layer (*HVL*) and tenth-value layer (*TVL*) were computed as a function of energy between 1 keV-100 GeV, while the atomic equivalent (Z_{eq}) and the buildup factors were calculated with 0.015 MeV-15 MeV energy range using Phy-X software. Moreover, all obtained values were compared with calculated ones using WinXCom program over the same energy range. Both calculation processes represent the μ_m reduction by following the energy increment. The Z_{eff} and N_{eff} show a similar trend depending on the energy range and have some discrete values at low energy. These discontinuous values correspond to the absorption edges which were also found in the μ_m calculation at same energy. The trends of *MFP*, *HVL*, and *TVL* are similar in that their highest values appear in the middle energy range with main interaction being Compton scattering. The buildup factors represent the multiple scattering of photons in materials and air with the main peaks in middle energy range.

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1. Introduction

The study of the interaction between photons and matter is fundamental in consideration of scintillator and phosphor materials [1]. The mass attenuation coefficient, effective atomic number, effective electron density, and cross-section are the essentially standard parameters used to develop and characterize new scintillation, phosphor and radiation shielding materials [2-5]. The interaction occurrence can be predicted using simulation in the WinXCOM program. Hubbell and Seltzer developed the program in 1995 that used a DOS system to calculate mass attenuation absorption by following the mixture rule of compounds. Gerward and his research group later developed the software from DOS to window system in the name of WinXCom [6]. There is another program, Phy-X, that can also simulate the interaction occurring in the 1 keV-100 GeV energy range in a similar way to WinXCom. Phy-X, created by E. Sakar and his research group, is user-friendly software for calculating the parameter values for radiation shielding, scintillation and dosimetry properties. Both software, WinXCom and Phy-X, can compute the interaction, absorption values, cross-sections, coherent scattering, incoherent scattering, photoelectric absorption, pairs production, half-value layer, tenth-value layer, and buildup factors, which are analyzed by the total mass attenuation coefficient's relation [7]. In 2016, Chewpraditkul and his colleagues [8] developed the $Gd_2YAl_2Ga_3O_{12}$:Ce crystal and measured its photoluminescence, energy resolution, light yield, and decay time. This substance has a high light yield, good energy resolution, and short scintillation decay time. The total mass attenuation coefficient (μ_m) energy of $Gd_2YAl_2Ga_3O_{12}$:Ce compound with 662 keV, which is essential property of a radiation detection material, was also studied. However, μ_m in the long energy range and other interaciton parameters composing of effective atomic number (Z_{eff}), effective electron density (N_{eff}), mean free path (*MFP*), half-value layer (*HVL*), tenth-value layer (*TVL*), and buildup factors of this compound have never been studied. Specifically, the buildup factors that determine how many interactions within the crystal or phosphor materials can occur. In $Gd_2YAl_2Ga_3O_{12}$:Ce, the photon interaction is prominent on the $Gd_2YAl_2Ga_3O_{12}$ host and it transfers the excitation energy to Ce dopant or even to other center of luminescence. It was fascinating to investigate the interaciton parameters of the $Gd_2YAl_2Ga_3O_{12}$ host compound for further development as a radiation detection material.

In light of this situation, the radiation interactions in the $Gd_2YAl_2Ga_3O_{12}$ compound were calculated and compared using two programs, the WinXCom and Phy-X software. The calculated parameters in this work included μ_m, Z_{eff}, N_{eff}, *MFP*, *HVL*, *TVL*, and buildup factors.

2. Materials and Methods

When a photon passes through matter, it can interact with the matter in three important ways such as the photoelectric, incoherent and pair production modes. The partial interaction summations are determined by the total mass attenuation coefficient, which is equal to a summation of the probabilities of those three interactions. The μ_m calculation follows the mixture rule of compounds, as seen in the following equation [9, 10];

$$\mu_m = \sum_i w_i \left(\mu_m\right)_i \tag{1}$$

where μ_m, w_i, and μ_i are the mass attenuation coefficient of a compound/mixture, weight fraction, and total mass attenuation coefficient of elements, respectively. The atomic ($\sigma_{t,a}$) and electronic ($\sigma_{t,el}$) cross-section can be computed from the μ_m value using the software and relations;

$$\sigma_{t,a} = \frac{\left(\mu_m\right)_{samples}}{N_A \sum_i^n \left(w_i / A_i\right)} \tag{2}$$

$$\sigma_{t,el} = \frac{1}{N_A} \sum_i^n \frac{f_i A_i \left(\mu_m\right)_i}{Z_i} \tag{3}$$

where N_A is Avogadro's number and A_i is atomic weight. Number of atoms of elements is in f_i symbol that relates to the total number of atoms of all elements, and Z_i is the atomic number of the element. The number of electrons per all atoms that interact with the photon can be determined in form of the effective atomic number.

$$Z_{eff} = \frac{\sigma_{t,a}}{\sigma_{t,el}} \tag{4}$$

From the relation of μ_m and $\sigma_{t,el}$, it can be used to evaluate the effective electron density by the equation;

$$N_{eff} = \frac{\mu_m}{\sigma_{t,el}} \tag{5}$$

The half-value layer, the thickness of specimen that reduces the radiation intensity to be half of the initial intensity, can be evaluated by the relation [9, 10];

$$HVL = \ln 2 / \mu \tag{6}$$

where μ is the linear attenuation coefficient by the relation of mass attenuation coefficients with material density.

The mean free path, the average path-length of photon that passes through the absorber materials before an interaction occurs, was calculated by the following relation [9, 10];

$$MFP = 1 / \mu \tag{7}$$

The tenth-value layer, the homogeneous material's thickness that can attenuate the radiation intensity to one-tenth, can be found from equation [9, 10];

$$TVL = \ln 10 / \mu \tag{8}$$

To calculate the atomic equivalent (Z_{eq}), it can first start from the incoherent/total attenuation absorption values calculated by the WinXCom program. The calculation is in the form of R function, and Z_1, Z_2 are the atomic numbers. The Z_{eq} can be computed from expression;

$$Z_{eq} = \frac{Z_1 \left(\log R_2 - \log R\right) + Z_2 \left(\log R - \log R_1\right)}{\log R_2 - \log R_1} \tag{9}$$

The G-P fitting values are computed from Be to Fe elements by the ANSI/ANS-6.4.3 (1991), an equation that can calculate the geometric progressions (G-P) fitting buildup factor;

$$P = \frac{P_1\left(\log Z_2 - \log Z_{eq}\right) + P_2\left(\log Z_{eq} - \log Z_1\right)}{\log Z_2 - \log Z_1} \tag{10}$$

The best equation for the gamma buildup factor representation relies on the G-P function which is in the form of [11, 12]

$$K\left(E,x\right) = px^a + d\frac{\tanh\left(x/Xk - 2\right)\tanh\left(-2\right)}{1 - \tanh\left(-2\right)} \quad \text{for (x)} \leq 40\text{mfp} \tag{11}$$

Finally, the equation of the buildup factor can be represented as follows:

$$B\left(E,x\right)1 + \frac{\left(\left(b-1\right)\left(k^X - 1\right) - \log Z_{eq}\right)}{k-1} \quad \text{for K} \neq 1 \tag{12}$$

3. Results and Discussion

3.1 Total mass attenuation coefficient

This work focused on the factors determining photon interactions of the $Gd_2YAl_2Ga_3O_{12}$ compound, the μ_m, Z_{eff}, N_{eff}, *MFP*, *HVL*, *TVL*, and the buildup factors. Those parameter values were compared by the calculations of the WinXCom and Phy-X programs, within 1 MeV-100 GeV energy range.

A comparison of calculated total mass attenuation coefficient between both software is exhibited in Figure 1. The μ_m tends to decrease with energy increasing between 10^{-3}-10^5 MeV. The energy's discontinuity in the low energy range of 10^{-3} MeV-10^{-1} MeV represents the absorption edge of K level of aluminum and gadolinium at 1.560 and 50.240 keV, respectively (shown in Table 1). The absorption edge values have a significant effect on the material's interactions. The calculation results from the WinXCom and Phy-X software are in good agreement and indicate the material's ability, which is the fundamental value for analysis in the light output of scintillator and phosphor materials.

3.2 Effective atomic number and effective electron density

Figure 2 shows the comparison of effective atomic number values from the WinXCom and Phy-X programs, which define the number of electrons per atom interacting with photons. The results indicate that there are more interactions at low energy than at high energy range, and the Z_{eff} values depend on the energy range. Furthermore, these values also represent the energy's discontinuity at the same position of the mass attenuation coefficients because of the absorption edges. The values of electron density obtained from WinXCom and Phy-X are demonstrated in Figure 3. The definition of N_{eff} is the number of electrons per gram that interacts with photons, and the calculation's results show the same trend with Z_{eff} values. Both N_{eff} and Z_{eff} values rely on the energy range and have discontinuous values at low energy, corresponding to the absorption edges at the same energy of the μ_m parameter.

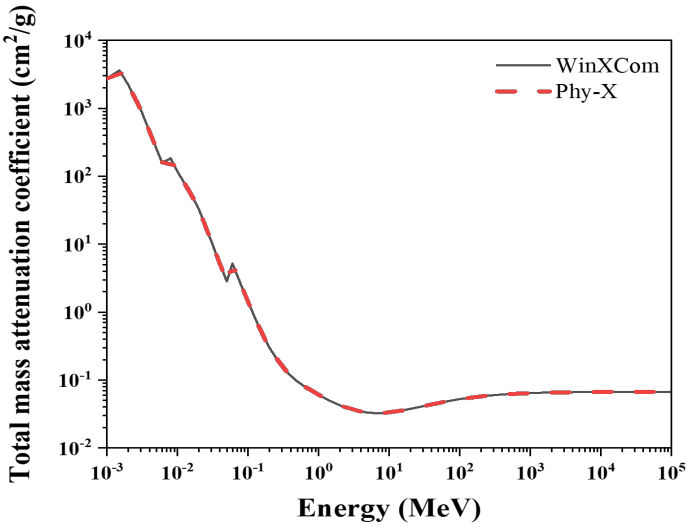

Figure 1. The mass attenuation coefficients (μ_m) calculated from WinXCom and Phy-X software

Table 1. The absorption edges (keV)

Elements	Z	M5	M4	M3	M2	M1	L3	L2	L1	K
Al	13	-	-	-	-	-	-	-	-	1.560
Ga	31	-	-	-	-	-	1.115	1.142	1.298	10.37
Y	39	-	-	-	-	-	1.020	1.043	1.194	17.04
Gd	64	1.185	1.217	1.544	1.688	1.881	7.243	7.930	8.376	50.24

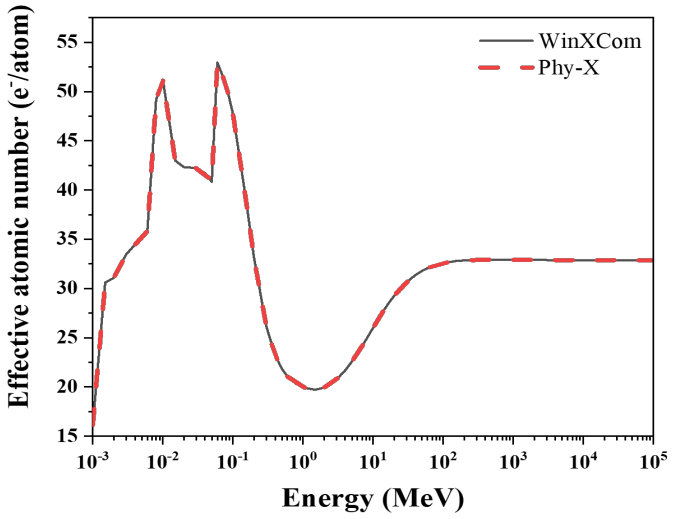

Figure 2. Effective atomic number (Z_{eff}) calculated from WinXCom and Phy-X software

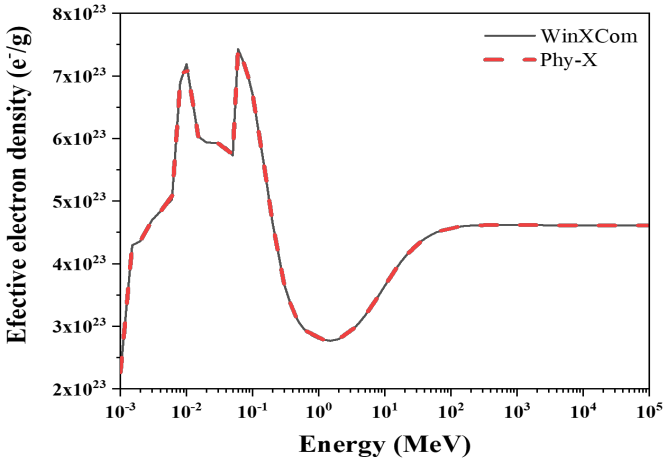

Figure 3. Effective electron density (N_{eff}) calculated from WinXCom and Phy-X software

3.3 Mean free path

The results for the average path-length, which refers to the path that photon can travel in materials before interaction occurrence, are shown in Figure 4. The computations show that the lowest *MFP* values are clearly located in the low energy region (10^{-3} MeV to 10^{-1} MeV). Afterwards, *MFP* slightly increases as it follows the energy increment and demonstrates its highest *MFP* values in the middle energy region with Compton scattering as the main interaction in this range. At higher energy than the point of maximum values, the *MFP* illustrate a continuous decrease with energy increment. These results indicate the variations in *MFP* in each energy range.

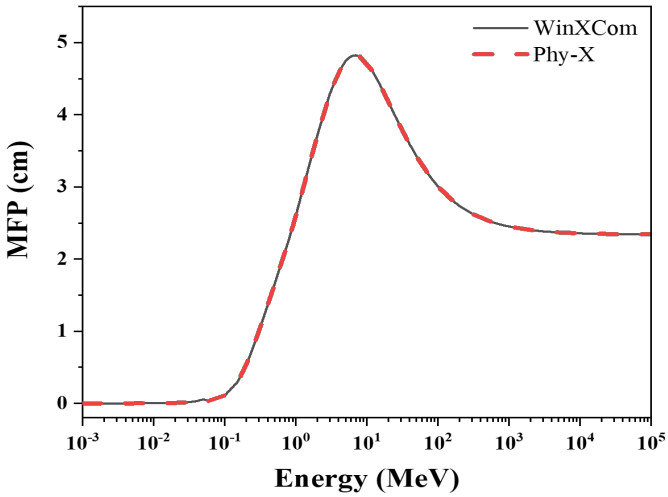

Figure 4. Mean free path (*MFP*) calculated from WinXCom and Phy-X software

3.4 Half-value layer and tenth value layer

Photon intensity decreases after propagating into more thickness of the specimen. The physical meaning of half-value layer is the thickness that decreases the intensity of radiation by half. The *HVL* can be evaluated using the relation in equation (6). Therefore, the specimens' *HVL* were plotted and compared between WinXCom and Phy-X programs, as shown in Figure 5. It was found that the lowest *HVL* values appear in low energy range, while the highest values are located in the middle energy range with the main interaction being Compton scattering. At energy higher than the point of maximum, the *HVL* decreases with energy increment, which corresponds with the *MFP* results mentioned previously. This can be explained that the photon energy is completely absorbed by main interaction of the photoelectric effect in low energy range, the *HVL* then is less able to reduce the radiation intensity to be half. For the middle energy range, at which the main interaction is Compton scattering, there remains the rest of photon energy after the interaction, which requires the high *HVL* of specimen to reduce that energy. In high energy range, pair production comes to play a role in the interaction and makes possible the absorption of some photon energy which results in the continuous reduction of *HVL* values. The results of tenth-value layers, which refers to the specimen thickness at which radiation intensity is reduced to one-tenth, are shown in Figure 6 and their explanations are similar to the *HVL*. The results for the two software programs are in good agreement, and suggest that the *HVL* and *TVL* variation depend on the energy range of incoming radiation.

3.5 The buildup factors

The variations of equivalent atomic number from WinXCom and Phy-X program are in good agreement and are shown in Figure 7. The Z_{eq} results demonstrate lower values at low and high ranges of energy. In the middle energy region, 0.1-1 MeV approximately, the Z_{eq} possesses the highest values because the Compton scattering is the primary interaction in this range. This leads to the determination of the exposure buildup factor (*EBF*) and energy absorption buildup factor (*EABF*).

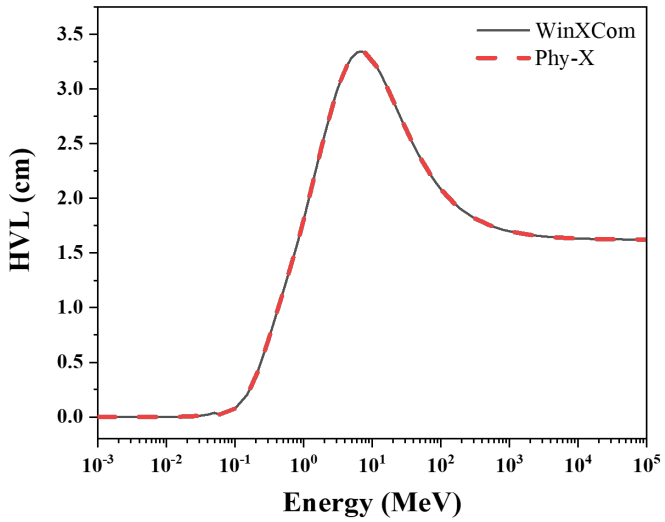

Figure 5. Half-value layers (*HVL*) calculated from WinXCom and Phy-X software

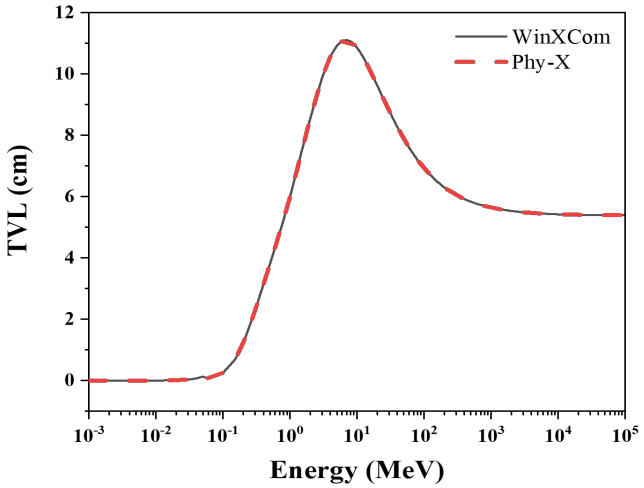

Figure 6. Tenth-value layers (*TVL*) calculated from WinXCom and Phy-X software

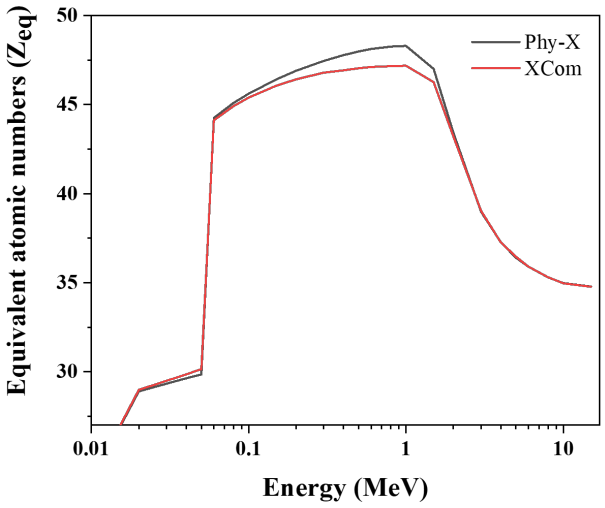

Figure 7. Equivalent atomic number (Z_{eq}) calculated from WinXCom and Phy-X software

In Figure 8, the *EABF* and *EBF* calculated by both programs increase with increasing mfp. The highest *EBF* and *EABF* values present at the enormous penetration depth of 40 mfp and they are explained by Compton phenomena at the middle energy range. In this range, the energy of photons will not be entirely removed, but will decreased. As a result, more multiple scattered photons will occur and affect the increasing of buildup in the material.

The *EABF* and *EBF* at 40 mfp calculated from both software programs were compared and are shown in Figure 9. It was found that *EBF* and *EABF* values show no significant differences in the high energy regions because of the tremendous *EABF* and *EBF* in materials. The *EBF* refers to the detector responsiveness corresponding to the attenuation in the air. It means that the exposure is

an absorption dose in the air. On the other hand, *EABF* shows the quantity of scattering energy and the function of responsive detectors for attenuation in the material. In the low energy range, the *EBF* of both programs are higher value than *EABF*, from which it can be concluded that the photon energy is more scattered from air into the detector than absorbed from the materials. For the middle energy region, the *EABF* values is slightly higher than *EBF* indicating that energy's absorption from the material is more prominent than absorption from the air. The *EBF* values are primarily considered for setting a suitable absorbed dose [11, 12] and they relate to the detector's abilities for radiation counting.

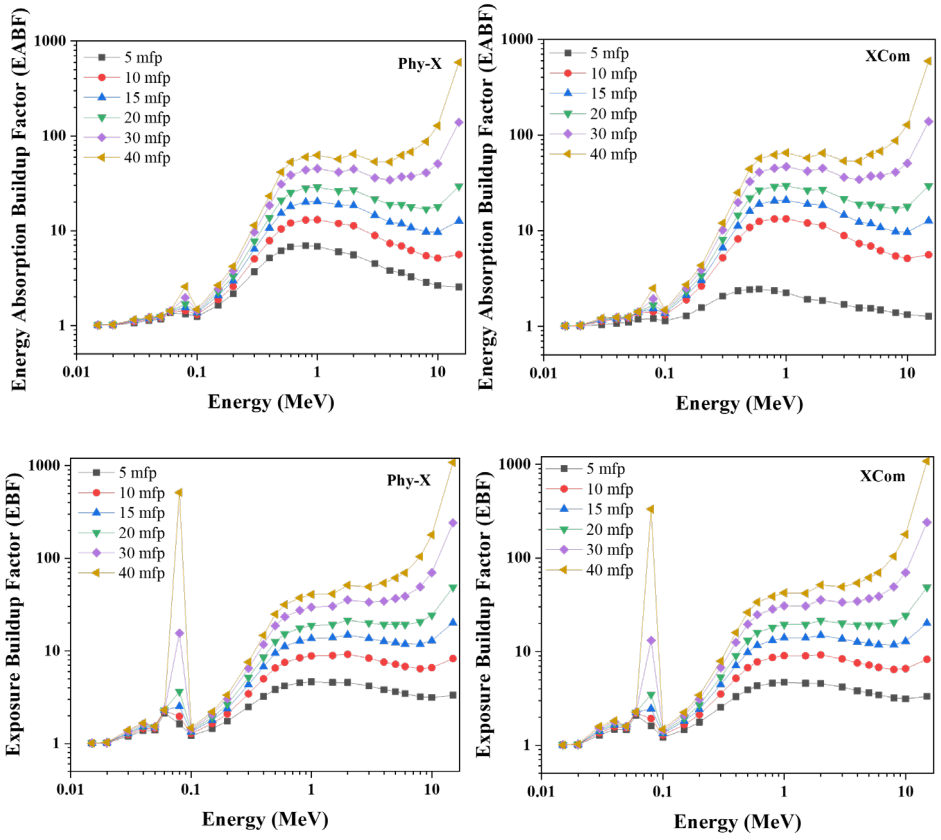

Figure 8. The energy absorption (*EABF*) and exposure (*EBF*) buildup factor calculated from Phy-X and WinXCom software

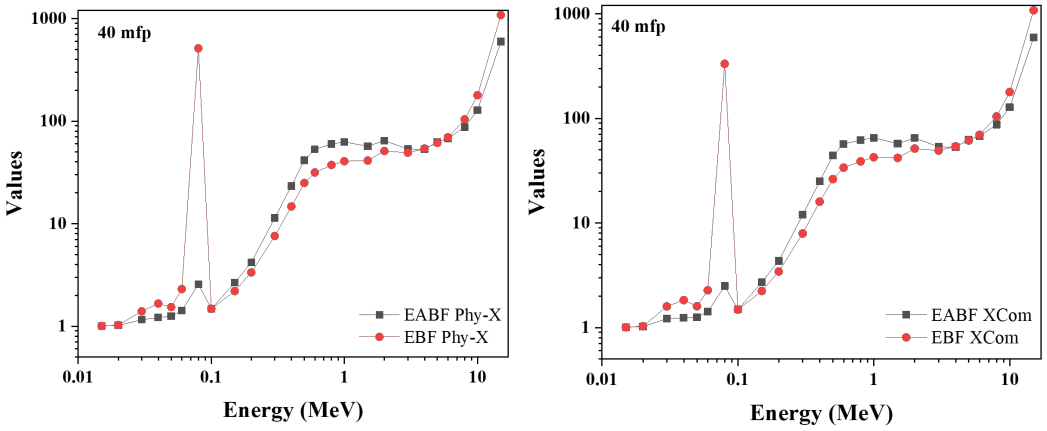

Figure 9. The comparison between energy absorption (*EABF*) and exposure (*EBF*) buildup factor with 40 mfp calculated from Phy-X and WinXCom software

4. Conclusions

The study of fundamental properties of photon interactions in the $Gd_2YAl_2Ga_3O_{12}$ compound by the μ_m, Z_{eff}, N_{eff}, *MFP*, *HVL*, *TVL*, and buildup factors were compared by use of the WinXCom and Phy-X programs. From the calculation in the energy ranges of 1 MeV-100 GeV and 0.015-15 MeV, it was found that the interaction parameter values depended on the energy of the photons. Moreover, the calculate values of fundamental interactions from both programs were in good agreement. These properties are the essential data used to determine the photon interactions and are necessary to predict the light output in scintillator and phosphor materials for radiation detection applications.

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