Simulation and theoretical evaluation of gamma radiation shielding efficiency of Phthalonitrile /WO_3 composites

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Introduction

Nowadays X-ray and gamma rays are being used within the domain of academics, accelerator facilities, radiation therapy, nuclear power plants, and industry for food irradiation. Exposure to gamma radiation has considerable health-related dangers. Considering their expense, accessibility, high density, and gamma-absorbing properties, lead-based materials are widely employed in radiation shielding; nonetheless, they have specific health and environmental risks [1-2]. Due to these problems, current developments have moved towards minimizing lead content in shielding from radiation. Polymer composites represent, however, a promising alternative, where high atomic number metal oxides are embedded in a polymer matrix, becoming more appropriate for gamma ray shielding [3].

The present work aims to study the radiation-shielding properties of tungsten trioxide (WO3) reinforced in a phthalonitrile (PN) polymer matrix using Geant4 Monte Carlo simulation and Phy-X/PSD software.

Phy-X/SD calculations and simulation

Phy-X/PSD (Photon Shielding and Dosimetry) is an online software available at https://phy-x.net/PSD. It serves as a platform for analyzing the shielding properties like LAC, MAC, MFP, HVL, TVL, etc. in the range of 1 keV to 100 GeV. The parameters are computed by entering the chemical formula of the composition in either mol% or wt% along with the density of the composites. Geant4 is a toolkit for simulation based on the Monte Carlo used in tracking radiation transmission through matter [3]. Geant4 code includes input files responsible for the sample and detector geometry, material's properties & compositions. Furthermore, the PhysicsList defines a particle i.e. gamma photon, and its interaction with the matter by the physics processes, namely the photoelectric effect, Compton scattering, and pair production. The simulations were done by modeling composite materials with seven different compositions. The density of the composite materials was assigned as per the theoretical calculations. A beam of Mono-energetic gamma photons (10^8) was randomly directed on the simulated material sample. The transmitted gamma photons were counted using a detector configured in the simulation framework. The energy of incident photons varied between 0.001 to 100 MeV. FTFP_BERT reference PhysicsList incorporated with G4EmLivermore Physics was used for the interactions of gamma photons with matter.

Materials and methods

Gamma radiation shielding properties of (100-*x*) $C_8H_4N_2$+$x$$WO_3$ composite, where x= 0, 5, 10, 20, 30, 40 and 50 wt% indicated as S1, S2, S3, S4, S5, S6 and S7. The density of the phthalonitrile matrix (PN) is 1.238 g/cm^3 and of WO_3 is 7.16 g/cm3. The density of the composites can be calculated using equation (1)

$$\rho_C = \frac{100}{\frac{100-w_{wo_3}}{\rho_{PN}}+\frac{w_{wO_3}}{\rho_{wO_3}}} \qquad (1)$$

Where, ρ_c, ρ_{PN} and ρ_{wo3} are the densities of the composite, phthalonitrile, and tungsten trioxide respectively, while W_{wo_3} is the weight fraction of tungsten oxides. The density (ρ_c) of the composites is given in **Table 1.**

Linear attenuation coefficients (μ_l) for seven samples of PN-WO_3 for the energy range

0.001-100 MeV were calculated by using incident intensity (I_0) and the reduced intensity (I) obtained by simulating the experiment in Geant4. Beer-Lambert's law gives the relation μ_l, I_0, and I as [2]:

$$\mu_l = \frac{\ln\left(\frac{I_0}{I}\right)}{x} \quad (2)$$

Mass attenuation coefficients (μ_m) were obtained by dividing the μ_l by the composite's density.

Table 1: The chemical composition of (100- *x*) $C_8H_4N_2$+ *x*WO_3 composite.

Sample code	Composition (wt %)		ρ_c gm/cm^3
	WO3	Phthalonitrile	
S1	0	100	1.380
S2	5	95	1.293
S3	10	90	1.352
S4	20	80	1.486
S5	30	70	1.649
S6	40	60	1.853
S7	50	50	2.114

Result and Discussion

The LAC and MAC calculated using Geant4 simulation were compared and validated with the data obtained using Phy-X/PSD software. The relative deviation between Geant4 and Phy-X/PSD results was calculated and deviation was found to be in the range of min 0.015% to max 12.89 %. The MAC obtained using Geant4 and Phy-X/PSD was plotted against the energy in **Fig. 1.** For energy from 1 keV up to 0.5 MeV, the MAC decreases sharply for all seven samples. This is because photoelectric absorption is dominant in this energy range. From 0.5 MeV energy, MAC decreases moderately due to the dominant effect of Compton scattering until 1.02 MeV. Above the energy 1.02 MeV, MAC was almost constant due to the dominance of the pair production effect.

The results also show that with increasing WO_3 content the MAC increases. However, with an increase in energy MAC decreases. This decrease is considerable in the low-energy region, due to the $Z^4/E^{3.4}$ dependence of photoelectric cross-section on atomic number (Z) and energy (E) [2]. The jumps observed in the plot shown in Fig. 1. for the samples on the addition of filler WO_3, are due to the absorption edges of tungsten (K, L, M edges).

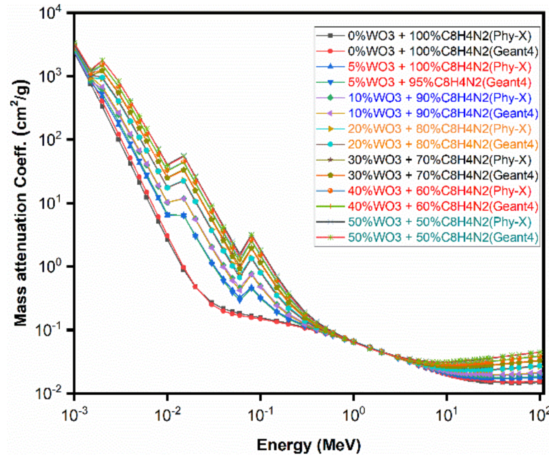

Fig.1 Comparison of mass attenuation coefficients for different compositions obtained by Geant4 code and Phy-X/PSD.

6. Conclusion

In the present investigation, Mass attenuation coefficients were calculated using Geant4 simulation and Phy-X/PSD software for different compositions of PN-WO_3 energies 0.001-100 MeV. The results are in close agreement and show strong radiation shielding ability in low-energy gamma fields.

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