

Evaluation of the Effect of Different Nanoparticles on the Mass Attenuation Coefficient of a Shield in Diagnostic Radiology: A Monte Carlo Study

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Abstract

Purpose: This research aimed to estimate the Mass Attenuation Coefficient (MAC) for the various nanoparticles in diagnostic imaging in order to assess and compare the changes in a bulk state.

Materials and Methods: To Using Monte Carlo N-Particle eXtended (MCNPX) code, nanoparticles were simulated in the target in order to compute the MAC considering the target. The Materials, including Bi, Pb NPs, Pb, W NPs, W, PbO NPs, Bi NPs, Bi₂O₃ NPs, and WO₃ NPs were used in the present study. The gathered data were compared with the theoretical results of the XCOM software for validation.

Results: The findings demonstrated that the radioprotective characteristics of nanoparticles in comparison to the bulk materials were better. Among all these nanoparticles, the rate of attenuation of tungsten nanoparticles was higher than that of other nanoparticles. On the other hand, the density and attenuation rate of nanoparticles of PbO, Bi₂O₃ and WO₃ were lower than those of nanoparticles Pb, W, and Bi. Therefore, all of the abovementioned nanoparticles were lightweight and their design was more flexible than that of bulk materials.

Conclusion: It was concluded that the use of nanoparticles in the protective materials considerably increased the radioprotective characteristics in the diagnostic radiography energy range.

Keywords: Mass Attenuation Coefficient; Nanoparticles; Monte Carlo; Radiology.

1. Introduction

Nowadays, with advances in nanotechnology and access to nanomaterials, this technology was considered a novel method to enhance the effectiveness of the conventional shielding utilized in the radiation protection field. Numerous studies have shown that the attenuation of photons of energy more than 1 MeV depends on the particle size of the filler materials [1]. Meanwhile, several studies have demonstrated that composites comprising of micro- and nanoparticles of high- Atomic number fillers dispersed in a conformable polymer matrix can be employed to design high-energy radiation shields which can be considered as an alternative to traditional shielding material [2-5].

The findings of these studies revealed that a smaller size of oxides doped into glassy materials can result in higher attenuation features. In addition, some micro- and nanoparticles adding to glass, concrete or other materials led to the identification of novel shielding protection materials which possess interesting absorption ability of the ionizing radiation [6-9]. According to the basic assumption of studies, the use of nano-particles produces more uniform distribution inside the matrix in comparison with microparticles, and thus higher photon attenuation would be achieved. The studies conducted on the epoxy composites filled with WO₃ micro- and nanoparticles provided a promising result for improved shielding effectiveness of nanoparticles [10-12].

Several investigations have been performed to investigate the radioprotective characteristics of materials containing the various elements in different energies (including Cu, Ba, Sn, W, Sn, Y, Gd, Pb and Zr). The nanomaterials applied in previous studies exhibit properties, including high density and an appropriate K-absorption edge for the used photon energy. The previous studies advised using elements like tungsten $Z = 74$ and bismuth $Z = 83$ instead of lead, because of the lower toxicity and cost-effectiveness [10, 12, 13].

Moreover, tungsten is identified as a high-Z metal having a lower density than lead which can reduce secondary radiation. Furthermore, the micro/nano-sized tungsten can lead to decreased weight because of its desirable dispersion in the matrix (increased surface-to-volume ratio). Various studies have also demonstrated that metallic fillers like Tungsten trioxide (WO₃) embedded in the Poly Vinyl Alcohol (PVA) polymer can

increase physical thermal, mechanical, optical, and electrical properties compared to its macro scales [14-20].

Given the properties of nanoparticles, this study aimed to estimate the effect of different nanoparticles on the Mass Attenuation Coefficient (MAC) of the shield in comparison with the bulk state using the Monte Carlo simulation code.

2. Materials and Methods

In the present study, Monte Carlo N-Particle eXtended (MCNPX) code (version.2.7.0) was employed to simulate Monte Carlo. The below-mentioned materials were used in this study: Pb, PbO Nano Particles (NPs), W, W NPs, Pb NPs, Bi, Bi NPs, WO₃ NPs, and Bi₂O₃ NPs. This simulation was done in three modes: bulk, pure nanoparticles (Pb, W, and Bi), as well as nanoparticles of WO₃, PbO, and Bi₂O₃.

The data collected from the simulation results were compared with the data of XCOM software for validation. This software can be used to calculate photon cross-sections for scattering, photoelectric absorption, and pair production, as well as total attenuation coefficients, for any element, compound, or mixture ($Z \leq 100$), at energies from 1 keV to 100 GeV. The XCOM program can generate cross-sections on a standard energy grid (spaced approximately logarithmically), or on a grid selected by the user, or for a mix of both grids. Cross-sections at energies immediately above and below all absorption edges are automatically included. XCOM provides two forms of output: (a) tables that correspond closely in format to existing tables in the literature; (b) a graphical display of the tabular data. The interaction coefficients and total attenuation coefficients for compounds or mixtures are obtained as sums of the corresponding quantities for the atomic constituents. The weighting factors, that is, the fractions by weight of the constituents, are calculated by XCOM from the chemical formula entered by the user. For mixtures, however, the user must supply the fractions by weight of the various components.

As shown in Figure 1, the narrow beam geometry such as source, collimators, and detector was modeled. In the current study, the narrow beam situation was reordered as a 60°-angle cone source which was placed 50 cm away from the shield. The source was considered a cone beam to make the program more effective and better geometry was obtained by 50 cm shield-detector distance [21]. The

shield was observed as a $10 \times 10 \times 0.1 \text{ cm}^3$ plate of shield materials.

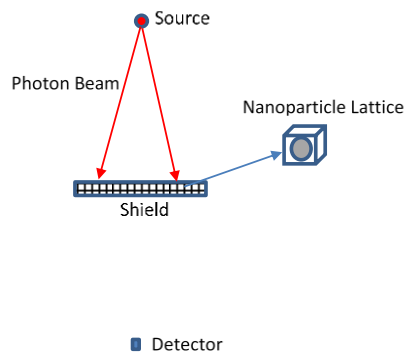


Figure 1. Schematic diagram for the geometry of the simulated beam and lattice-universe arrangement containing nanoparticles

In this simulation, the radiant energy ranged from 10 to 100 keV.

In this study, the nano-sized fillers were as follows: lead (Pb, $K = 88 \text{ keV}$), tungsten (W, $K = 69.5 \text{ keV}$), and bismuth (Bi, $K = 90.5 \text{ keV}$). These particles exhibited a relatively high atomic number and density. Accordingly, we tested these nanoparticles and assessed their performance as shielding nanocomposites individually and as MCNP samples in the energy range of 10-100 keV. The Monte Carlo method was employed to calculate the attenuation coefficient of the above-mentioned nanoparticles. Each nanoparticle was situated as a sphere having a diameter of 50 nm in the center of the voxels. In addition, nanoparticles WO_3 , PbO , and Bi_2O_3 were used in order to reduce weight more.

For simulation, spherical NPs filled by uniformly shield mass were used. The dimensions of the spherical NPs were $2 \times 2 \times 2 \text{ mm}^3$. For cubic and octagonal prismatic networks, Lattice (LAT) = 1 and LAT = 2 Cards were utilized, respectively. For defining the cell, the given cards are used together with Filled (FILL) and Universe (U) cards. A world can be considered a regular or normal network of cells. Similar to that given to the card FILL of the cell, the non-zero value entered for card U. Card FILL showed that the desired cell was filled by the cells possessing card U.

The output data was determined by the f4 tally, representing the flux of photons passing through a cell. The duration of each simulation was about 15 hours in order to reduce the error. During this time, about 2 billion photons with various energies were observed and tracked

by the simulator. The following equation was applied to compute the MAC of the various samples (Equation 1):

$$MAC = \frac{1}{\rho \cdot x} \cdot \ln \left(\frac{I_0}{I} \right) \quad (1)$$

Where MAC stands for Mass Attenuation Coefficient, I and I_0 represent the Intensity in the presence and absence of an absorber, respectively, x (cm) denotes the thickness of the absorbing material, and ρ ($\text{g} \cdot \text{cm}^{-3}$) represents the density of the material used.

The results obtained from the simulations for the samples were compared with those of the XCOM program so as to confirm the accuracy of the findings.

3. Results

The MACs of lead, bismuth, and tungsten at the photon energies of 10-100 keV were computed and compared by the data obtained from the National Institute of Standards and Technology (NIST) [22]. As depicted in Figures 2, 3, and 4, a close agreement was observed between the results of MC and the data obtained from NIST. A maximum difference of 2% was detected between the values obtained from MC and NIST. Thus, in the present study, the MC model was validated for further simulations. As shown in Figures 2-4, the MACs of lead, bismuth, and tungsten in the bulk state were compared with their nano state, respectively. As can be seen in these figures, the mass attenuation rate is now greater than the bulk state. The maximum difference between these two states (nano and bulk Pb) was obtained at an energy of 100 keV. This value was 1.70 times higher for the nano mode than for the bulk mode (Figure 2). The maximum difference between these two states (nano and bulk Bi) was obtained at an energy of 40 keV. This value was 1.72 times higher

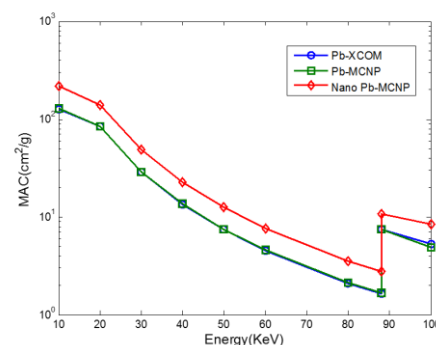


Figure 2. The computational Mass Attenuation Coefficient (MAC) obtained for Bulk and Nano Lead as a function of energy. In bulk mode, the simulation data and the data obtained from the XCOM software almost coincide

for the nano mode than for the bulk mode (Figure 3). The maximum difference between these two states (nano and bulk W) was obtained at an energy of 70 keV. This value was 2.44 times higher for the nano mode than for the bulk mode (Figure 4).

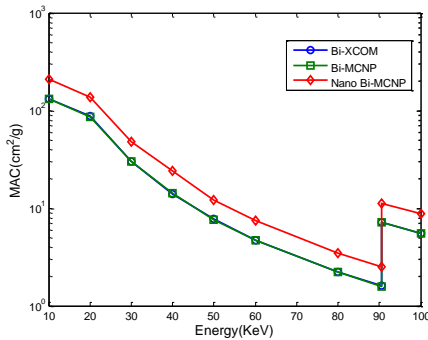


Figure 3. The computational MAC of Bulk and Nano Bismuth as a function of energy. In bulk mode, the simulation data and the data obtained from the XCOM software almost coincide

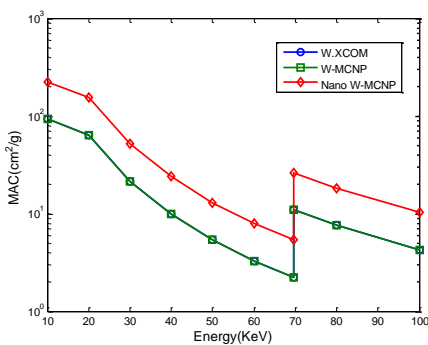


Figure 4. The computational MAC of Bulk and Nano Tungsten as a function of energy. In bulk mode, the simulation data and the data obtained from the XCOM software almost coincide

Figure 5 shows the MAC for the three nanomaterials of lead, bismuth and tungsten. As can be seen in this figure, the MAC for tungsten nanoparticles, in the energy range of 70 to 88 keV, is higher than the other two nanomaterials. Figure 6 shows MAC of nano shield samples (such as PbO, Bi₂O₃, and WO₃).

4. Discussion

The majority of recent studies have demonstrated that the incorporation of nanomaterials in composites can lead to the efficient absorption and attenuation of radiation. In the present study, nanoparticles were used instead of bulk material to design non-lead shields. The characteristics

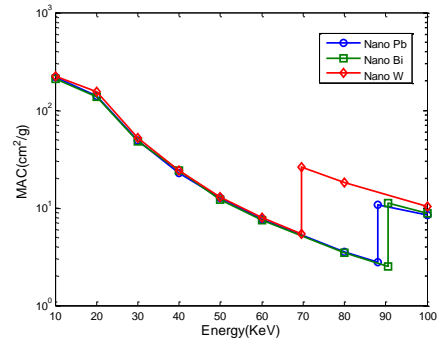


Figure 5. MAC for Nano Lead, Nano Bismuth & Nano tungsten were obtained of MCNP code. These data are obtained from Figures 2, 3, and 4

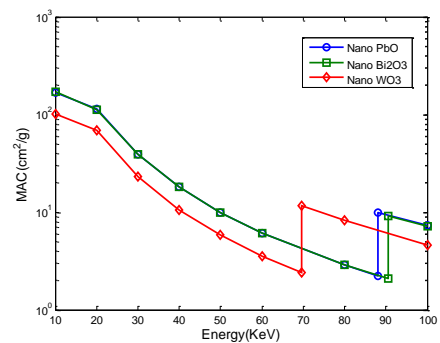


Figure 6. MACs for Nano PbO, Nano Bi₂O₃ & Nano WO₃ were obtained of MCNP code

of nanoparticles are such that they are very low in weight and due to that can provide a good attenuation for medium energies in the X-ray spectrum [23]. After extensive simulations, the combinations, including PbO, Bi₂O₃, and WO₃ were finally obtained that were better than the other compounds in terms of the higher attenuation. Nano-shields of PbO, Bi₂O₃, and WO₃ had less weight and were more flexibility than nano-materials of Pb, Bi, and W [9].

On the other hand, due to economic reasons and availability, samples that include PbO, WO₃, and Bi₂O₃ can be introduced as a cost-effective composite than other multiple samples [24]. Using appropriate composite materials with different K-absorption edges provides dominance of the photoelectric effect to Compton scattering in beam absorption and leads to a reduction in weight with equivalent protection. Indeed, X-rays would be absorbed several times by multiple K- absorption edges.

At energies less than 69 keV, the attenuation rates of nanoparticles of, PbO, and Bi₂O₃ were slightly higher than that of WO₃ nanoparticles. The reason for this phenomenon can be due to the higher atomic number of lead and bismuth compared to tungsten. In energies between 69 to 88 keV, the attenuation coefficient of the composites doped with

nano-WO₃ was enhanced in the energy range of 69.5 keV, which might be due to the specific absorption at the K-absorption edge energy of WO₃ and an increase in the protective properties of the shield [11]. Our results indicated that nanoparticles of Bi₂O₃ and WO₃ had better attenuation relative to lead shield materials.

5. Conclusion

In conclusion, the use of WO₃, PbO, and Bi₂O₃ nanoparticles in shielding material exhibited higher photon attenuation in comparison with bulk materials. The sample containing WO₃ and Bi₂O₃ showed greater shielding effectiveness in the photon energy range of 10-100 keV. The current study recommends that nanoparticles can be used to fabricate novel shielding materials for medical application of photons.

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