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Investigation of two heavy element scintillators by Monte-Carlo methods

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ABSTRACT: The aim of this study was to estimate the influence of K-characteristic radiation on the performance of x-ray scintillating screens containing two heavy elements by Monte Carlo methods. K-characteristic radiation is produced within materials of at least one heavy (high atomic number) element. This radiation may result either in spatial resolution degradation or in emission efficiency decrease. The scintillators studied were the following: LYSO (Lu_{1.8}Y_{0.2}SiO₅ and LuYSiO₅), CsI and YTaO₄. All the aforementioned scintillators have two heavy elements, thus the K-characteristic radiation of the high-Z element can produce additional K-characteristic photons on the low-Z element, resulting in further degradation. Scintillator performance was described in terms of the: (a) Probability of generation and reabsorption of a K-characteristic photon (PKR) and (b) Spatial distribution of K-characteristic radiation within the scintillator material. A custom validated Monte Carlo model was used, in order to simulate the transport of K-characteristic radiation within the above scintillator materials. Results showed that, depending on screen thickness (20–100 mg/cm²) and incident photon energy (20–80 keV) the scintillator's emission efficiency may be significantly reduced.

KEYWORDS: X-ray detectors; Detector modelling and simulations I (interaction of radiation with matter, interaction of photons with matter, interaction of hadrons with matter, etc)

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Contents

1 Introduction	1
2 Materials and methods	1
3 Results and discussion	2
4 Conclusion	4

1 Introduction

Scintillators or phosphor screens are used as x-ray to light converters in radiation detectors of a large variety of medical imaging applications. LYSO ($\text{Lu}_{2(1-x)}\text{Y}_{2x}\text{SiO}_5$), CsI and YTaO_4 are scintillators containing two heavy ($Z > 30$) elements (i.e. Lu and Y in LYSO, Cs and I in CsI, Y and Ta in YTaO_4). Heavy elements, through photoelectric absorption of incident x-rays, may produce intrinsically generated (or secondary) radiation, i.e. K-characteristic x-ray photons of considerably high energy ($E > 10$ keV). Many works, investigating the effect of K-characteristic radiation in x-ray imaging detectors, have been published [1–4]. In these studies, analytical or Monte Carlo models were developed estimating the fraction of the reabsorbed K x-rays. According to our knowledge, the effect of K-characteristic photon production on the performance of LYSO scintillator has never been previously investigated by Monte Carlo methods.

In the present study, a previously developed (in MATLAB) custom validated Monte Carlo simulation program [5–7] has been extended, in order to investigate the K-characteristic effect (in terms of absolute or relative values and in terms of spatial distribution) on scintillators with two K-absorption edges.

2 Materials and methods

In the present work, a custom Monte Carlo simulation code was utilized [5–7]. The latter requires as input data, the x-ray energy or spectrum, the phosphor material’s chemical composition and some standard reference tabulated data related to the phosphor material’s physical parameters [8–11]. This simulation code was developed by performing an account of the energy deposition, which contributes to light generation, from the x-ray photon interactions in the diagnostic energy range. This account included the elastic and inelastic scattering effects as well as the photoelectric effect.

The proposed Monte Carlo model was applied to investigate parameters related to K-characteristic effect on the aforementioned scintillators. LYSO scintillator is a mixed LSO/YSO ($\text{Lu}_2\text{SiO}_5/\text{Y}_2\text{SiO}_5$) scintillator. The ratio of LSO/YSO may vary from 50/50 up to 90/10. For brevity reasons, in this study only the two limiting ratios for LYSO scintillator were investigated. The coating thickness of phosphor screens was varying from 20 up to 100 mg/cm².

Table 1. Physical properties of the investigated scintillators related to the K-characteristic radiation.

<i>Scintillator</i>	<i>Heavy element</i>	<i>K-edge (keV)</i>	ω_K	<i>Average energy (keV)</i>
LYSO	Lu (71) Y (39)	63.31 17.04	0.9487 0.7155	53.79 14.89
CsI	Cs (55) I (53)	35.98 33.17	0.8942 0.8819	30.89 28.51
YTaO ₄	Y (39) Ta (73)	17.04 67.42	0.7155 0.9522	57.22 14.89

The incident radiation beam was assumed to be mono-energetic, consisting of 10^6 x-ray photons, following pencil beam geometry, with energy in the range 20–80 keV. Energies within this range were used for simulation of conditions used in x-ray mammography and in general x-ray radiography [12].

When an incident photon interacts with the scintillator material one of the following physical processes may occur: (i) *Photoelectric Effect* or (ii) *Compton Scattering* or (iii) *Raleigh Scattering*. In the case that Photoelectric Effect occurs, photoelectric absorption takes place either in the K or in the L-shell of the interacting element. In the first case, K-characteristic photons are produced according to the corresponding K-fluorescent yield ω_K [13]. Their energies are just below the photoelectric K-absorption edge. Therefore, a K x-ray photon may travel through the absorbing material at a distance called free path length (fpl), which is proportional to its energy. Hence, these photons may either escape the scintillator or be absorbed at various sites in the scintillator. The Monte Carlo simulation program took into consideration the production of two K-characteristic photons (K_1 and K_2) with different energies, for each heavy element. The average energy was calculated by means of the relative frequency, I_y , of K_1 or K_2 production [13]. It may be observed that K-characteristic radiation of the high-Z element can produce additional K-characteristic photons on the low-Z element, resulting in further degradation. Table 1 shows some relevant data.

The probability of generation and reabsorption of a K x-ray (PKR), was calculated as the fraction of reabsorbed K x-ray photons with respect to the initially produced K x-ray photons. This parameter shows the tendency of a K x-ray photon to be reabsorbed within the scintillator. The spatial distribution of the absorbed K x-ray photons energy is another useful parameter. It shows the K x-ray photons effect on image blurring, i.e. in the spatial resolution degradation. The scintillator slab was partitioned into 50 small areas. The number of the K x-ray photons absorbed within each area was calculated. The corresponding absorbed energy was then determined by summing the number of absorbed K x-ray photons of a specific element multiplied by the photon energy.

3 Results and discussion

Figure 1 shows the probability of K x-ray photons reabsorption within LYSO 50/50 and LYSO 90/10 scintillators. More specifically, it depicts the reabsorption probability for the K x-ray photons produced on Lu atoms (K_Lu), the K x-ray photons of Y, due to the incident primary x-ray photons (K_Y/inc), and the K x-ray photons of Y due to interaction of the K x-ray photons originating from Lu (K_Y/Lu). It may be observed that the PKRs of the low-Z element (such as Y) are higher than that of the high-Z element (i.e. Lu). This happens because the K x-rays of Y have lower energy and consequently lower tendency to escape the scintillator.

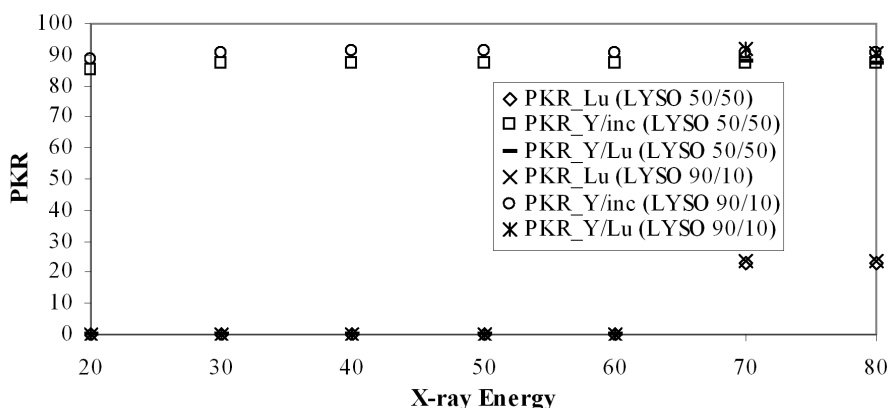


Figure 1. Probability of K x-ray photon reabsorption versus x-ray energy for 60 mg/cm^2 of LYSO.

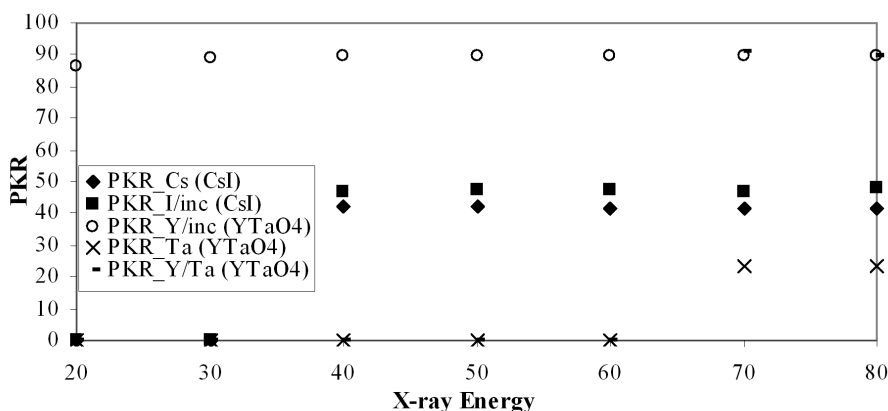


Figure 2. Probability of K x-ray photon reabsorption vs x-ray energy for 60 mg/cm^2 of CsI and YTaO₄.

In this energy range, PKRs have almost constant values. This happens because the average energies of K x-ray photons of both Lu and Y have accurately fixed energies, regardless of the incident x-ray photon energy. In the case of LYSO 90/10, the PKRs of Y/inc and Y/Lu decrease in comparison with the PKR corresponding to LYSO 50/50. This takes place because the fraction of Lu increases, so there is an increased probability for the K x-ray photons of Y to interact with the L-shell electrons of the Lu atoms. Figure 2 shows the probability of K x-ray photons reabsorption within CsI and YTaO₄ scintillators. In this case, PKRs of Y have the highest values, while that of Ta have the lowest. It was found that K x-ray photons of Cs cannot produce additional K x-ray photons to I element. This occurs because their energy (30.89 keV) is lower than the K absorption edge energy of I (33.17).

Figure 3 shows the spatial distribution of the absorbed K x-ray photon energy for 60 mg/cm^2 of all the investigated scintillators. The considered energy of incident x-ray beam for each scintillator was chosen to be close to its high-Z element K-edge (i.e. 65 keV for LYSO, 40 keV for CsI and 70 keV for YTaO₄). This consideration was made in order to investigate the highest effect of K x-rays on image blurring. It may can be seen that LYSO 50/50, LYSO 90/10 and YTaO₄ scintillators

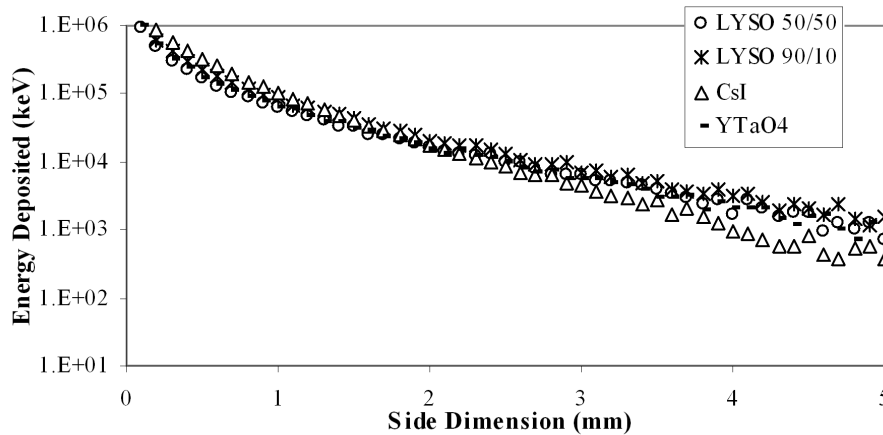


Figure 3. Spatial distribution of the absorbed K x-ray photon energy for 60 mg/cm^2 of all scintillators

have almost the same spatial distribution. This occurs because of the presence of Lu (53.79 keV) and Ta (57.22 keV) elements, respectively. CsI scintillator has higher values at low distances and lower values at higher distances in comparison with the previous scintillators. This happens because its elements emit K x-ray photons of lower energy (30.89 and 28.51 keV). Therefore, they are absorbed more locally.

4 Conclusion

Using this model, it was found that the K-characteristic photons produced by the higher atomic number element of the scintillator (e.g. Lu inside LYSO) show a higher tendency to escape the scintillator. This is because heavier elements produce K x-ray photons with higher characteristic energy, so they have larger penetrating ability. Therefore, phosphors containing heavy elements with comparatively low-Z (such as CsI scintillator), absorb a larger fraction of the produced K x-ray photons than phosphors with high-Z heavy elements. However, high-Z element scintillators may absorb a slightly higher number of K x-ray photons in comparison with that of low-Z scintillators, under the same conditions (e.g. comparison between LYSO 90/10 and LYSO 50/50). This happens because, in the first case, scintillators absorb a higher amount of the incident x-ray photons, resulting in a higher production of K x-ray photons.

In the case that the K x-rays produced in high-Z heavy elements are reabsorbed, this occurs at relatively large distances away from the point of their creation. Hence, their lateral diffusion is larger. This may result in image blurring effects which may extend to a wide range.

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