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INVESTIGATION OF SCINTILLATORS WITH TWO K-ABSORPTION EDGES USING MONTE CARLO TECHNIQUES.

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MASTER THESIS

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To my family

To my sister’s family

To my niece, Archontoula Papalaskari
# TABLE OF CONTENTS

ABSTRACT ............................................................................................................................................. 8  
A. INTRODUCTION .................................................................................................................................. 9  
   A.1 The problem ................................................................................................................................. 10  
   A.2 Thesis Originality ...................................................................................................................... 11  
   A.3 Publications .............................................................................................................................. 11  
B. THEORETICAL PART ............................................................................................................................ 13  
   B.1 X-rays ........................................................................................................................................ 14  
      B.1.1 Nature of X-rays .................................................................................................................. 14  
      B.1.2 X-ray production .................................................................................................................. 14  
   B.2 γ-rays (gamma rays) ..................................................................................................................... 15  
      B.2.1 Nature and production of γ-rays ....................................................................................... 15  
   B.3 X or γ-ray interactions with matter ............................................................................................ 16  
      B.3.1 Photoelectric absorption ...................................................................................................... 16  
         B.3.1.1 K-characteristic radiation .............................................................................................. 17  
      B.3.2 Compton (incoherent) scattering ....................................................................................... 18  
      B.3.3 Rayleigh (coherent) scattering ............................................................................................ 20  
      B.3.4 Pair production ..................................................................................................................... 20  
   B.4 Attenuation coefficients ................................................................................................................. 21  
      B.4.1 Total linear attenuation coefficient .................................................................................... 21  
      B.4.2 Total mass attenuation coefficient ..................................................................................... 22  
      B.4.3 K, L or M-edges ................................................................................................................... 22  
      B.4.4 Attenuation for compounds .................................................................................................. 23  
   B.5 Scintillators in x and γ-ray imaging: An overview ..................................................................... 24  
      B.5.1 Introduction .......................................................................................................................... 24  
      B.5.2 X-ray imaging ....................................................................................................................... 24  
      B.5.3 γ-ray imaging ....................................................................................................................... 25  
   B.6 The quest for the ideal scintillator ................................................................................................ 25  
      B.6.1 Introduction .......................................................................................................................... 25  
      B.6.2 Physical and luminescent characteristics of a scintillator ...................................................... 26  
      B.6.3 K-characteristic effect on scintillators .................................................................................. 26  
      B.6.4 Investigated scintillators ......................................................................................................... 27  
      B.6.5 Attenuation coefficients of scintillators ............................................................................... 30  
      B.6.6 Investigated performance of the scintillators ...................................................................... 35  
         B.6.6.1 Quantum Detection Efficiency (QDE) ........................................................................... 35  
         B.6.6.2 The number of produced K x-ray photons ................................................................. 36  
         B.6.6.3 The number of reabsorbed K x-ray photons ................................................................. 36  
         B.6.6.4 K-factor ........................................................................................................................ 37  
         B.6.6.5 Probability of K-fluorescence x-ray photon generation per Absorbed x-ray (PKA) ................... 37  
         B.6.6.6 Probability of K-fluorescence x-ray photon generation per Incident x-ray (PKI) ........ 38  
         B.6.6.7 Probability of generation and Reabsorption of a K x-ray per incident x-ray (PKR) .... 38  
         B.6.6.8 Spatial distribution of the absorbed K x-ray photons (number and energy) .................... 40
C. MONTE CARLO METHODS .........................................................................................................................41
   C.1 Introduction ...........................................................................................................................................42
   C.2 Sampling techniques .............................................................................................................................44
      C.2.1 Inverse method ..............................................................................................................................44
      C.2.2 Acceptance-Rejection method ......................................................................................................45
D. MATERIALS AND METHODS-THE MONTE CARLO MODEL ...............................................................46
   D.1 Geometry of the simulation ....................................................................................................................47
   D.2 Simulation of the x-ray photon history inside the scintillator ...............................................................47
      D.2.1 Photoelectric absorption ................................................................................................................48
      D.2.2 Compton scattering .......................................................................................................................49
      D.2.3 Rayleigh scattering .......................................................................................................................49
   D.3 Input data required to the Monte Carlo program ..................................................................................50
   D.4 Calculated output parameters by the Monte Carlo program ...............................................................50
   D.5 Average absolute relative difference between Monte Carlo and theoretical values ................................51
E. RESULTS AND DISCUSSION ....................................................................................................................53
   E.1 Quantum Detection Efficiency (QDE) ....................................................................................................54
   E.2 The number of produced and absorbed K x-ray photons .......................................................................62
   E.3 K-Factor ..................................................................................................................................................74
   E.4 Probabilities for K x-ray photons (PKA, PKI and PKR) ........................................................................80
   E.5 Spatial distribution of the absorbed K x-ray photons (number and energy) .........................................88
F. CONCLUSIONS AND FUTURE WORK ....................................................................................................93
   F.1 Conclusions ..........................................................................................................................................94
   F.2 Future work .........................................................................................................................................95
APPENDIX I: ABBREVIATIONS .....................................................................................................................96
REFERENCES ....................................................................................................................................................97
ABSTRACT

The performance of phosphor screens (or scintillators) used in medical imaging systems are strongly affected by the intrinsic phosphor properties. The present study investigates scintillator radiation detection efficiency and how the produced K-characteristic radiation affects scintillator performance. K-characteristic radiation may either be reabsorbed or it may escape the scintillator. In both cases the imaging performance of the scintillator may be affected resulting either in spatial resolution degradation or in counting efficiency decrease. Scintillator employed in medical imaging detectors may have either one heavy element (e.g. Lu in LSO) or two heavy elements (e.g. Lu and Y in LYSO). In the latter case, further image degradation may result, since K x-rays of the high-Z element can produce additional K-characteristic radiation to the low-Z element. In the present study two scintillators with one heavy element (LSO, YSO) and three with two heavy elements (LYSO, CsI and YTaO₄) were investigated. The study was carried out by the extension of a previously developed custom and validated Monte Carlo simulation program. When possible, Monte Carlo results were compared to analytical models.

The study was made under conditions used in general x-ray radiography, x-ray mammography, CT and nuclear medicine γ-ray imaging (γ-camera and SPECT). Therefore, a monoenergetic x-ray beam was assumed, varying in the range from 20 up to 160 keV. The respective scintillator thickness was considered to vary from 20 up to 100 mg/cm². Results showed that K characteristic effect of additional K x-ray photons is negligible on thin phosphor screens, while it is considerably higher in thicker scintillators. In addition, it was found that YSO scintillator is suitable for use in x-ray mammography. On the other hand, LSO, LYSO, CsI and YTaO₄ scintillators were found suitable for higher energy imaging applications.
CHAPTER A

INTRODUCTION

A.1 The problem .................................................................................................................................................. 10
A.2 Thesis Originality ......................................................................................................................................... 11
A.3 Publications .................................................................................................................................................. 11
A.1 The problem

Luminescent materials or scintillators are employed as radiation to light converters in detectors of medical imaging systems (conventional and digital x-ray radiography, mammography, x-ray Computed Tomography (CT), Positron Emission Tomography (PET) and Single Photon Emission Computed Tomography (SPECT)) (Johns and Cunningham 1983, Yaffe 2000). In x-ray projection imaging, a large number of such materials have been employed in the form of granular screens (Blaše and Grabmaier 1994), often referred to as phosphor screens. Phosphor screens consist of a large number of grains embedded within a binding material. The x-ray detection and imaging performance of these materials are affected by intrinsic physical properties, related to x-ray and light photon transport through the material. These properties have been previously investigated 1) experimentally (Van Eijk 2001, Dick and Motz 1981a, Venema 1979) 2) theoretically (Venema 1979, Chan and Doi 1983a, Nishikawa and Yaffe 1990, Kandarakis et al 1997) and 3) by Monte Carlo models (Raeside 1976, Morin 1988, Andreo 1991, Kalender 1981, Chan and Doi 1983b). The investigation of these properties has been taken into account in the design of commercial imaging systems (Yaffe and Rowlands 1997, Van Eijk 2002).

Phosphor screens are materials which usually consist of two or three (in some cases four) elements. In the case of at least one heavy (high atomic number) element, K-characteristic (fluorescence) radiation is produced. This type of radiation may carry a considerable fraction of initially absorbed radiation, which may either be reabsorbed or it may escape the scintillator. In both cases the imaging performance of the scintillator may be affected resulting either in spatial resolution degradation or in counting efficiency decrease. Many works, investigating the effect of K-characteristic radiation on x-ray imaging detectors, have been published. In these studies, analytical-theoretical (Venema 1979, Chan and Doi 1983 a, Kalivas et al 1999, Kandarakis et al 2003, Kandarakis et al 2005, Kandarakis et al 2006) or Monte Carlo methods (Chan and Doi 1984, Boone et al 1999, Liaparinos et al 2006 a) were developed estimating the fraction of the re-absorbed K X-rays. Many scintillators are consisted of two heavy elements. Therefore, K-characteristic radiation of the high-Z element can be absorbed by the K-absorption edge of the low-Z element, producing secondary K-characteristic photons to the low-Z element. This results in further image quality degradation. The effect of two heavy element scintillator’s K-fluorescence on the detection and imaging performance has been widely investigated by analytical-theoretical methods (Chan and Doi 1983 a). On the other hand, according to our
knowledge only a few relative parameters have been investigated by Monte Carlo methods (Boone et al 1999).

A.2 Thesis Originality

The originality of this thesis consists of:

- The extension of a previously developed custom and validated Monte Carlo simulation program (Liaparinos et al 2006 b, Liaparinos et al 2007, Liaparinos 2007). This extension was made 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 (i.e. LYSO (Lu$_{2(1-x)}$Y$_{2x}$SiO$_5$), CsI and YTaO$_4$). When possible, Monte Carlo results were compared to analytical models.

- 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.

- Some probabilities concerning K x-ray photons (PKA, PKI and PKR) of scintillators with two K-absorption edges, have never been previously investigated by Monte Carlo methods.

A.3 Publications

This work resulted in publications in national and international conferences.

Publications in international scientific conference proceedings with referees


Abstracts in international scientific conferences


Abstracts in national scientific conferences

• Α. Κωνσταντινίδης, Π. Λιαπαρίνος, Γ. Παναγιωτάκης και Ι. Κανδαράκης “ΜΕΛΕΤΗ ΤΗΣ ΕΠΙΔΡΑΣΗΣ ΤΗΣ Κ-ΧΑΡΑΚΤΗΡΙΣΤΙΚΗΣ ΑΚΤΙΝΟΒΟΛΙΑΣ ΣΕ ΣΠΙΝΘΗΡΙΣΤΕΣ ΙΑΤΡΙΚΗΣ ΑΠΕΙΚΟΝΙΣΗΣ ΜΕ ΧΡΗΣΗ ΤΕΧΝΙΚΩΝ ΜΟΝΤΕ CARLO”, 17ο Διαπανεπιστημικό Συνέδριο Ακτινολογίας 2007, 9-11 Νοεμβρίου 2007, Πάτρα.
CHAPTER B

THEORETICAL PART

<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>B.1 X-rays</td>
<td></td>
<td>14</td>
</tr>
<tr>
<td>B.1.1</td>
<td>Nature of X-rays</td>
<td>14</td>
</tr>
<tr>
<td>B.1.2</td>
<td>X-ray production</td>
<td>14</td>
</tr>
<tr>
<td>B.2 γ-rays (gamma rays)</td>
<td></td>
<td>15</td>
</tr>
<tr>
<td>B.2.1</td>
<td>Nature and production of γ-rays</td>
<td>15</td>
</tr>
<tr>
<td>B.3 X or γ-ray interactions with matter</td>
<td></td>
<td>16</td>
</tr>
<tr>
<td>B.3.1</td>
<td>Photoelectric absorption</td>
<td>16</td>
</tr>
<tr>
<td>B.3.1.1</td>
<td>K-characteristic radiation</td>
<td>17</td>
</tr>
<tr>
<td>B.3.2</td>
<td>Compton (incoherent) scattering</td>
<td>18</td>
</tr>
<tr>
<td>B.3.3</td>
<td>Rayleigh (coherent) scattering</td>
<td>20</td>
</tr>
<tr>
<td>B.3.4</td>
<td>Pair production</td>
<td>20</td>
</tr>
<tr>
<td>B.4 Attenuation coefficients</td>
<td></td>
<td>21</td>
</tr>
<tr>
<td>B.4.1</td>
<td>Total linear attenuation coefficient</td>
<td>21</td>
</tr>
<tr>
<td>B.4.2</td>
<td>Total mass attenuation coefficient</td>
<td>22</td>
</tr>
<tr>
<td>B.4.3</td>
<td>K, L or M-edges</td>
<td>22</td>
</tr>
<tr>
<td>B.4.4</td>
<td>Attenuation for compounds</td>
<td>23</td>
</tr>
<tr>
<td>B.5 Scintillators in x and γ-ray imaging: An overview</td>
<td></td>
<td>24</td>
</tr>
<tr>
<td>B.5.1</td>
<td>Introduction</td>
<td>24</td>
</tr>
<tr>
<td>B.5.2</td>
<td>X-ray imaging</td>
<td>24</td>
</tr>
<tr>
<td>B.5.3</td>
<td>γ-ray imaging</td>
<td>25</td>
</tr>
<tr>
<td>B.6 The quest for the ideal scintillator</td>
<td></td>
<td>25</td>
</tr>
<tr>
<td>B.6.1</td>
<td>Introduction</td>
<td>25</td>
</tr>
<tr>
<td>B.6.2</td>
<td>Physical and luminescent characteristics of a scintillator</td>
<td>26</td>
</tr>
<tr>
<td>B.6.3</td>
<td>K-characteristic effect on scintillators</td>
<td>26</td>
</tr>
<tr>
<td>B.6.4</td>
<td>Investigated scintillators</td>
<td>27</td>
</tr>
<tr>
<td>B.6.5</td>
<td>Attenuation coefficients of scintillators</td>
<td>30</td>
</tr>
<tr>
<td>B.6.6</td>
<td>Investigated performance of the scintillators</td>
<td>35</td>
</tr>
<tr>
<td>B.6.6.1</td>
<td>Quantum Detection Efficiency (QDE)</td>
<td>35</td>
</tr>
<tr>
<td>B.6.6.2</td>
<td>The number of produced K x-ray photons</td>
<td>36</td>
</tr>
<tr>
<td>B.6.6.3</td>
<td>The number of reabsorbed K x-ray photons</td>
<td>36</td>
</tr>
<tr>
<td>B.6.6.4</td>
<td>K-factor</td>
<td>37</td>
</tr>
<tr>
<td>B.6.6.5</td>
<td>Probability of K-fluorescence x-ray photon generation per Absorbed x-ray (PKA)</td>
<td>37</td>
</tr>
<tr>
<td>B.6.6.6</td>
<td>Probability of K-fluorescence x-ray photon generation per Incident x-ray (PKI)</td>
<td>38</td>
</tr>
<tr>
<td>B.6.6.7</td>
<td>Probability of generation and Reabsorption of a K x-ray per Incident x-ray (PKR)</td>
<td>38</td>
</tr>
<tr>
<td>B.6.6.8</td>
<td>Spatial distribution of the absorbed K x-ray photons (number and energy)</td>
<td>40</td>
</tr>
</tbody>
</table>
**B.1 X-rays**

**B.1.1 Nature of X-rays**

X-ray (or Roentgen) radiation consists of electromagnetic waves, like light, radiophone, telephone and television waves. The difference between X-ray radiation and the latter waves is that it has very small wavelength. Because of this characteristic, x-rays have high penetrative ability between the materials. Therefore, they are used in x-ray imaging for human organs’ investigation. Electromagnetic radiation is not continuous energy fluence, but a sequence of non-continuous energy packages. Each energy package is known as photon or quantum. The energy of each photon increases as a function of electromagnetic radiation’s frequency $\nu$ by the following formula:

$$E = h \cdot \nu$$

where $h$ is Planck’s constant ($h = 4.135 \times 10^{-15} eV \cdot s$)

The frequency of every electromagnetic radiation is inversely proportional of the wavelength as shown above:

$$c = \lambda \cdot \nu \Rightarrow \lambda = c / \nu \text{ and } \nu = c / \lambda$$

where $c$ is light’s speed ($c = 3 \times 10^8 m/s$) and $\lambda$ is electromagnetic radiation’s wavelength (Boone 2000).

**B.1.2 X-ray production**

X-rays are produced when rapidly moving electrons strike a solid target inside the x-ray tube and their kinetic energy is converted into radiation. The wavelength of the emitted radiation depends on the energy of the electrons. X-rays were first discovered in 1895 by Wilhelm Conrad Roentgen, who was awarded the 1901 Nobel Prize in physics for this achievement.

X-ray radiation production stems from electrons that have been accelerated in vacuum from the cathode to the anode of an x-ray tube. Electrons emission occurs when a filament is heated by current passing through it. When the filament is hot enough, the electrons obtain thermal energy sufficient to overcome the energy binding the electron to the metal of the filament. After being accelerated, they are stopped by the anode at a short distance. Most of the electron energy will produce heat at the anode. Some percentage will be converted to x-ray by two physical mechanisms: brake (or Bremsstrahlung) and characteristic radiation.
1. Brake (or Bremsstrahlung) radiation

According to the classical theory, deceleration of charged particle results in the emission of electromagnetic field. When moving electrons strike a metallic target, as the anode, they interact with the electrostatic field of its atomic nucleus and they decelerate. If their interaction is far from the nucleus, they give a small fraction of their kinetic energy. The produced x-ray radiation has relatively low energy, while electrons have high kinetic energy and may interact with following target atoms. On the other hand, it is highly unlikely for them to interact very close to the nucleus, so they can give all their kinetic energy to the produced x-rays. Consequently, the produced x-rays will have a wide, continuous distribution of energies with the maximum being the total energy that the electron had when reaching the anode. The number of x-rays will be small at lower energies and increased for higher energies.

2. Characteristic radiation

It is the result of moving electrons interaction with the peripheral electrons of target’s atoms. According to the classical model of Bohr about the atom, electrons are at certain quantum energy shells (K, L, M etc). Electrons of each shell have a prescribed and approximately equal binding energy with regard to the nucleus. Inner shells electrons (K, L) have higher binding energies than those of the outer shells (M, N etc). If a moving electron impinges with an inner shell (e.g. K-shell) electron, the latter is removed from its orbit, leaving a vacancy. An electron from an outer shell (e.g. L or M-shell) shifts into the inner shell’s vacancy in order to fill it. The product of this transition is electromagnetic (i.e. x-ray) radiation, having energy equal to the energy difference between the two shells.

B.2 γ-rays (gamma rays)

B.2.1 Nature and production of γ-rays

γ-rays are electromagnetic waves (such as x-rays), emitted from the inside of the atomic nucleus. Radioactive nuclei (or isotopes) are fission into daughter isotopes, emitting α or β radiation. However, daughter isotopes remain usually in excited state. They go into fundamental situation, emitting one or more γ-ray photons. Frequency and energy of γ-ray photons have characteristic values for specific nucleus. These values are determined by the following equation (Κανδαράκης 1994 b):

\[ E_γ = E_1 - E_2 = h \cdot ν \]  

(3)
where $E_1$ is the energy of the initial excited situation, $E_2$ is the energy of the new situation, $\nu$ and $h\nu$ are emitted photon’s frequency and energy, respectively. $\gamma$-ray photons’ energies are usually higher than that of x-ray photons.

Also, a $\gamma$-ray photon can be produced through the phenomenon of annihilation. Two 511 keV photons are emitted oppositely directed when a positron, emitted by a relative radiopharmaceutical, annihilates. However, this phenomenon is out of the present investigation’s interest.

B.3 X or $\gamma$-ray interactions with matter

These interactions in general can result in energy deposition and, in many cases a secondary x-ray will be present after the initial interaction. Some products of these interactions are scattered x-rays, characteristic x-rays, and annihilation radiation. The four basic x or $\gamma$-ray interactions with matter are the Photoelectric absorption, Rayleigh scattering, Compton scattering and Pair production.

B.3.1 Photoelectric absorption

Photoelectric absorption is the interaction of an incident x or $\gamma$-ray photon with an inner shell (K or L-shell) electron of the absorbing atom. The basic prerequisite for this interaction to take place is that the incident photon’s energy must be higher than the binding energy of the electron. During the absorption, the incident x-ray photon transfers its energy to the electron and results in the ejection of the electron from its shell (usually the K-shell) with a kinetic energy equal to the difference of the incident photon energy $E_0$ and the electron shell binding energy $E_{BE}$. The created vacancy is subsequently filled by an electron from an outer shell with less binding energy (e.g. from the L or M-shell). The energy difference between these two shells can be emitted either 1) as an x-ray photon (K, L or M-characteristic or fluorescence radiation in proportion with the respective shell) or 2) transferred to an electron of the same atom. If this difference is larger than the binding energy of the electron, the latter becomes free (Auger effect).
If the incident photon energy is less than the binding energy of the electron, the photoelectric interaction cannot occur. On the other hand, if it is equal to the electronic binding energy \( (E_0 = E_{BE}) \), the photoelectric effect becomes energetically feasible and a large increase in attenuation occurs (K, L or M absorption edge). As the incident photon energy increases above that of the electron shell binding energy, the photoelectric absorption probability \( \tau \) decreases at a rate proportional to \( 1/E^3 \). Also, the photoelectric absorption probability is proportional to the atomic number of the absorber \( (\sim Z^3) \). After photoelectric interaction, ionization of the atom occurs and a free electron and a positively charged atom are produced. Kinetic energy (motion) of the ejected photoelectron can cause further electron-electron ionization, with most energy locally deposited. Also, a subsequent cascade of electron transitions filling the vacated inner electron shell results in emission of characteristic radiation (Boone 2000, Seibert and Boone 2005).

**B.3.1.1 K-characteristic radiation**

K-characteristic (or fluorescence) radiation takes place because of the electrons’ transitions (or relaxations) from outer shells \( (L, M \) or \( N \)-shells) to K-shell of an element’s atom. Each shell is composed of certain sub-shells \( \text{(i.e. } L\text{-shell consists of } L_1, L_2 \text{ and } L_3 \text{ sub-shells, } M\text{-shell consists of } M_1, M_2, M_3, M_4 \text{ and } M_5 \text{ sub-shells etc.)} \). The most probable atom relaxations are K-L2, K-L3, K-M2, K-M3, K-N2 and K-N3. However, in the present study only K-L2 and K-L3 relaxations were taken into consideration. The corresponding K-characteristic radiation is called \( K_\alpha \) (or \( K_1 \)) and \( K_\beta \) (or \( K_2 \)) fluorescence. Their energies equal to the difference of binding
energies between K–shell and L2 or L3 sub-shells respectively. The relative frequency, $I_y$, of either a K\(\alpha\) or K\(\beta\) fluorescence x-ray photon production is not the same. In most elements the value of $I_\alpha$ is close to 0.35 (35%), while $I_\beta$ is almost 0.65. For heavy (high atomic number, i.e. $Z>30$) elements K-characteristic radiation occurs at relatively high energies ($E>10$ keV). This happens because the binding energy of K-shell electrons (i.e. the K-absorption edge energy) is proportional to the atomic number of the element. Due to the fact that in heavy elements K-characteristic radiation has not negligible energies (>5 keV), this radiation energy isn’t absorbed locally. 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. On the other hand, L or M characteristic x-ray photons are considered to be locally absorbed, because their energy is too low. K, L or M x-ray photons may be emitted isotropically at all directions.

A relative parameter to K-characteristic radiation is the K fluorescence yield, $\omega_K$. It expresses the ratio of the average number of K-fluorescence x-rays produced over the number of vacancies created in the K-shell (Auger electrons excluded). For instance, if $\omega_K=0.7$, there is 70 % possibility for K-fluorescence x-rays production and 30 % possibility for Auger electron release.

According to the above theory, it may be observed that K-characteristic x-ray photons’ energies of an element have rates lower than the K absorption edge energy of the same element. Therefore, it is not possible to produce additional K-characteristic radiation at the same element. However, if a material consists of two heavy elements, K-characteristic radiation energies of the heaviest element (highest $Z$) may have higher values than the K absorption edge energy of the low-$Z$ element. This effect leads to the production of additional K x-ray radiation originating from the low-$Z$ element (Chan and Doi 1983 a, Liaparinos et al 2006 a, Kandarakis et al 2006).

### B.3.2 Compton (incoherent) scattering

Compton scattering, also known as incoherent scattering, contributes to the attenuation of x or $\gamma$-rays in matter. It occurs when an incident x-ray photon strikes and ejects a free or loosely bound electron from an atom. During this interaction a fraction of incident photon energy is provided as kinetic energy to the atomic electron. The rest energy remains to the photon, which after the interaction change its propagation directory (it is scattered). The angle of the new direction (in relation with the initial) is called scattering angle. Supposing the struck electron is
at rest and neglecting its binding energy, the energy transferred to the electron $E_e$ can be found using energy and momentum conservation:

$$E_e = E_{\gamma} \frac{m_0 c^2}{1 + \frac{E_{\gamma}}{m_0 c^2}(1 - \cos \theta)}$$

where $m_0$ is rest mass of electron, $c$ is the speed of light, $E_{\gamma}$ is the initial photon energy and $\theta$ is the scattering angle of the scattered photon. It may be observed that $E_e$ is proportional to the scattering angle. The change in wavelength of the scattered photon is given by:

$$\lambda_s - \lambda_p = \frac{h}{m_0 c}(1 - \cos \theta)$$

where $h$ is the Planck’s constant. (Seibert and Boone 2005, Κανδαράκης 1994 a)

Compton scattering probability $\sigma$ is proportional to electrons number per mass unit and density of the absorbent material. Finally, it is independent from the absorbent material’s atomic number $Z$. 

![Figure 2: Compton scattering](image)
B.3.3 Rayleigh (coherent) scattering

An incident x-ray photon can interact with an electron and be deflected (scattered) with no loss in energy. This process is also known as coherent or elastic scattering, and it occurs by temporarily raising the energy of the electron without removing it from the atom. The electron returns to its previous energy level by emitting an x-ray photon of equal energy but with a slightly different direction. Most x-rays are scattered forward by this mechanism, because the atom cannot experience significant recoil without otherwise removing the electron. There is no absorption of energy, and the majority of the x-ray photons are scattered with a small angle. The probability of Rayleigh scattering is indicated by the symbol $\sigma_{\text{COH}}$ or $\sigma_R$. In soft tissue, the probability of this event occurring is low, on the order of ~5% of all scattering events, because of the low effective atomic number of soft tissues ($Z \sim 7.5$). The possibility of Rayleigh scattering increases with increasing $Z$ of the absorbent material and decreasing x-ray energy (Seibert and Boone 2005, Κανδαράκης 1994 a).

![Rayleigh scattering](image)

Figure 3: Rayleigh scattering

B.3.4 Pair production

Pair production can occur when the incident x-ray photon has energy greater than 1.02 MeV, which represents the rest mass energy equivalent of 2 electrons (i.e., $E = 2 \cdot m_0c^2$, where $m_0$ is the rest mass of the electron ($9.11 \cdot 10^{-31}$ kg) and $c$ is the speed of light ($3.0 \cdot 10^8$ m/s)). The interaction of the incident photon with the electric field of the nucleus results in the production of an electron ($e^-$) and a positron ($e^+$) pair, with any photon energy in excess of 1.02 MeV being
transferred to the kinetic energy of the e\(^-\)/e\(^+\) pair equally. Interestingly, ionization of the atom does not occur, although charged particles are formed and their kinetic energy can result in subsequent ionization within the local area. Once the positron expends its kinetic energy, it combines with any available electron and produces annihilation radiation, resulting from the conversion of the rest mass energies of the e\(^-\)/e\(^+\) pair into (nearly) oppositely directed 511 keV photons. The probability of pair production \(\pi\), increases with energy above 1.02 MeV. Though annihilation radiation is crucial for PET, pair production occurs at energies well above those used for diagnostic x-ray imaging (Seibert and Boone, 2005, Κανδαράκης 1994 a).

![Image of electron and positron](image)

**Figure 4:** Pair production

### B.4 Attenuation coefficients

#### B.4.1 Total linear attenuation coefficient

The interaction mechanisms discussed above, combine to attenuate the incident photon beam as it passes through matter. Attenuation is the removal of x or \(\gamma\)-ray photons from their beam either by absorption or scattering events. For a monoenergetic beam of \(N_0\) photons incident on a thin slab of material of thickness \(x\) with a probability of attenuation \(\mu\), the fractional reduction of the number of photons from the beam is constant. An exponential relationship exists between the incident and transmitted photon fluence (number of photons/mm\(^2\) area) after passing through a total material thickness \(x\) of the attenuating material as described by the following equation:

\[
N_x = N_0 e^{-\mu x}
\]
where $\mu$ is the total linear attenuation coefficient, which represents the probability of attenuation per unit of thickness of the material. The unit of thickness $x$ is commonly expressed in centimetres, so the corresponding unit of $\mu$ is cm$^{-1}$. The total linear attenuation coefficient is the sum of the linear attenuation coefficients for the individual interaction mechanisms, as:

$$\mu = \tau + \sigma + \sigma_R + \kappa$$  \hspace{1cm} (7)

where $\tau, \sigma, \sigma_R$ and $\kappa$ are the Photoelectric absorption, Compton scattering, Rayleigh scattering and Pair production linear attenuation coefficients correspondingly. Like the above individual interaction coefficients, values of $\mu$ are strongly dependent on incident x-ray energy and on the physical density of the interacting medium. (Berger et al 1999).

**B.4.2 Total mass attenuation coefficient**

At a given photon energy, the linear attenuation coefficient can vary significantly for the same material if it exhibits differences in physical density (e.g. water, water vapour and ice). The total mass attenuation coefficient $\mu/\rho$, compensates these variations by normalizing the linear attenuation with the density of the material. Therefore, the mass attenuation coefficients for water, water vapour, and ice are identical. For the total mass attenuation coefficient, “thickness” becomes the product of the density (g/cm$^3$) and linear thickness (cm) of the material, or $\rho x$. This is known as coating thickness with units of (g/cm$^3$)·cm=g/cm$^2$. The reverse value of the mass thickness represents the units of total mass attenuation coefficient (cm$^2$/g). The corresponding equation is:

$$N_x = N_0 e^{-\left(\frac{\mu}{\rho}\right)\rho x}$$  \hspace{1cm} (8)

Like the total linear attenuation coefficient, the total mass attenuation coefficient for a specific material is the sum of the respective individual interaction probabilities (Seibert and Boone 2005, Κανδαράκης 1994 a, Berger et al 1999):

$$\frac{\mu}{\rho} = \frac{\tau}{\rho} + \frac{\sigma}{\rho} + \frac{\sigma_R}{\rho} + \frac{\kappa}{\rho}$$  \hspace{1cm} (9)

**B.4.3 K, L or M-edges**

It is observed that both total linear and mass total attenuation coefficients of the materials present sudden increases (peaks) of their values at certain energies. These energies are the respective electronic binding energies of K, L or M shells of the atoms of the elements which constitute the materials. If the incident photon energy is less than the binding energy of a
certain shell’s electron, the photoelectric interaction cannot occur. On the other hand, if it is equal to the electronic binding energy ($E_0 = E_{BE}$), the photoelectric effect becomes energetically feasible. At diagnostic energies up to 160 keV, which are used in the present study, photoelectric effect is the fundamental interaction. Therefore a large increase in total attenuation coefficient occurs. These sudden increases are called K, L or M-edges (or absorption edges).

The K absorption edge refers to the sudden increase in the probability of photoelectric absorption when the K-shell interaction is energetically possible. Similarly, the L or M absorption edges refer to the sudden increases in photoelectric absorption occurring at the L or M-shell electron binding energies respectively (at much lower energies).

**B.4.4 Attenuation for compounds**

Attenuation coefficients for compounds (materials comprised of 2 or more elements) can be determined as the weighted average (by mass) of the individual mass attenuation coefficients of the compound’s constituent elements, as:

$$\left( \frac{\mu}{\rho} \right)_{\text{compound}} = \sum_{i=1}^{N} m_i \left( \frac{\mu}{\rho} \right)_i$$

(10)
where \( m_i \) is the mass fraction (fraction of the element’s mass contribution to the total mass) and \( (\mu/\rho)_i \) is the mass attenuation coefficient of element \( i \) in the compound. This is important for estimating attenuation probabilities of compounds and materials that cannot be easily measured and particularly for computer simulations (Seibert and Boone 2005).

**B.5 Scintillators in x and \( \gamma \)-ray imaging: An overview**

**B.5.1 Introduction**

Scintillators (or phosphor screens or phosphors) convert x or \( \gamma \)-ray radiation into optical photons (Κανδαράκης 1994 a). They are employed in most of the current medical diagnostic imaging modalities using x or \( \gamma \)-rays (conventional and digital x-ray radiography, mammography, x-ray Computed Tomography (CT), \( \gamma \)-camera, Single Photon Emission Computed Tomography (SPECT) and Positron Emission Tomography (PET)). This is explained by the good detection efficiency of scintillators for hard radiation. Yet, the variously used diagnostic methods differ considerably. Consequently, the radiation requirements also differ. These requirements are not always met by the scintillator specifications. New, digital diagnostic systems with an excellent image quality and a short image acquisition time and excellent quality real-time imaging systems for interventional radiology at a low radiation dose, are two main reasons for continuous scintillator search (Johns and Cunningham 1983, Knoll 1989).

**B.5.2 X-ray imaging**

In x-ray radiography (static imaging) an attenuation profile of a part of the human body is projected onto a two-dimensional position-sensitive radiation detector (PSD) using the focus of an x-ray tube as a point source. Thus, information on anatomical detail is obtained. A variety of radiation detectors are used. For example, at present, for chest radiography x-ray phosphor-screen-film cassettes, typically of 35x43 cm\(^2\), are applied as the PSD on a large scale. In most cases Gd\(_2\)O\(_2\)S:Tb is used as the x-ray intensifying screen phosphor. Furthermore, a digital chest-radiography system is used based on the electrostatic read-out of a drum covered with an amorphous-selenium (a-Se) semiconductor layer as the PSD. Recently, new digital radiography (DR) systems have been introduced employing an a-Se photoconductor layer deposited on top of an amorphous-silicon (a-Si:H) thin-film transistor array or employing a Gd\(_2\)O\(_2\)S:Tb phosphor screen deposited on top of an array of a-Si:H photodiodes coupled to an array of thin-film transistors. In mammography film-screen cassettes of 18x24 cm\(^2\) are generally used. In
this case a resolution of 0.1 mm is required to observe micro calcifications. Conventional film-screens systems usually consist of two equal phosphor-binder layers (thickness up to 0.3 mm per layer) and two equal emulsion layers, one on each side of the film base. More advanced systems for chest radiography are asymmetric in structure, i.e. the two screens have different thicknesses and the two emulsions are of different contrast. In mammography only one relatively thin screen (0.07 mm) and one emulsion are used to realize the required resolution (Van Eijk 2002, Yaffe and Rowlands, 1997).

B.5.3 \(\gamma\) -ray imaging

In radionuclide imaging based on single-photon emission, the gamma radiation emitted by a radiopharmaceutical introduced into the body is used either for simple projections (planar scintigraphy) or for single-photon emission computed tomography (SPECT) (Webb 1990). In both cases gamma cameras are used, originally typically circular with a diameter up to 50 cm, employing a monolithic NaI:Tl crystal plate (thickness 6–12 mm) and photomultiplier tube (PMT) read-out (e.g. hexagonal packing of 61 PMTs). In positron emission tomography (PET), imaging is realized by means of two 511 keV quanta which are emitted oppositely directed when a positron, emitted by a radiopharmaceutical introduced into a patient, annihilates in tissue. The two annihilation quanta are detected position sensitively in coincidence. To a good approximation, the point of positron emission is situated on the line of response connecting the two detection positions. Many annihilation events give many lines of response (LOR) and in principle the three-dimensional reconstruction of the LOR represents the radiopharmaceutical distribution, i.e. the image. For position-sensitive detection, a PET system consists, in general, of many rings with thousands of scintillation detectors (Van Eijk 2002).

B.6 The quest for the ideal scintillator

B.6.1 Introduction

Since the 1950’s many new inorganic scintillator materials have been invented. Also, the relative scientific community made advances in understanding the basic physical processes governing the transformation of ionizing radiation into scintillation light. Whereas scintillators are available with a good combination of physical properties, none of them provides the desired combination of stopping power, light output and decay time. Hence, accordingly to the use of a scintillator in medical diagnostic imaging system, scintillator should appear the desirable combination of fluorescence properties.
B.6.2 Physical and luminescent characteristics of a scintillator

The following scintillator’s characteristics are required for use in x or $\gamma$-ray imaging:

1. **Detection efficiency**: Detection efficiency expresses the scintillators’ ability to detect the incident radiation. High density is important for reducing the amount of scintillator material needed.

2. **Cost and physical form**: These factors are closely related with the ease of crystal growth, because the cost of growing the crystal growth is usually much higher than the cost of the raw materials. Crystals that do not decompose or undergo a phase transformation between room temperature and their melting point are the easiest to produce in large shapes at low cost.

3. **Light yield**: Whereas high light yield may not be too critical for detecting very energetic particles, increased light yield is important for improving accuracy and spatial resolution. Energy resolution also depends on light yield and proportionality.

4. **Peak emission’s wavelength**: The emission wavelength and the light yield will determine the best photodetector to use (e.g. photomultiplier tube, photodiode, avalanche photodiode).

5. **Decay time**: Decay time expresses how fast the light is emitted. Fast signal rise and decay times are important for good timing resolution and high counting rates. Decay time depends on activator (Knoll 1989, Κανδαράκης 1994 a).

For brevity reasons, $\gamma$-ray photons will be referred to as x-ray photons in the rest of this investigation.

B.6.3 K-characteristic effect on scintillators

As it was mentioned above, K-characteristic radiation is a product of photoelectric absorption between incident x-rays and K-shell electrons of heavy elements atoms. The produced K x-rays can travel to any direction. Their free path length is proportional to their energy. If they are reabsorbed inside the scintillator, they may produce light photons which do not correspond to incident x-ray beam, resulting in image blurring. If they escape the scintillator, they decrease the counting efficiency of the system. It is known that nuclear medicine imaging detectors measure counts. The number of accepted counts corresponds to those photons that have deposited all their energy within the scintillator. The counting efficiency of the system corresponds to the total number of counts accepted by the pulse-height
analyzer over the number of photoelectric events. The possible decrease in this efficiency was estimated by evaluating the loss of counts due to the amount of K-fluorescence x-ray photons escaping the scintillating crystal. In this case, counts of lower amplitude are produced, which normally are rejected by the pulse-height analyzer. There are scintillators with one heavy element (e.g. Lu inside LSO) and scintillators with two heavy elements (e.g. Lu and Y inside LYSO). The latter results to further image degradation, because K x-rays of the high-Z element can produce additional K characteristic radiation to the low-Z element.

**B.6.4 Investigated scintillators**

In the present study five scintillators (LSO, YSO, LYSO, CsI and YTaO₄) were investigated using Monte Carlo methods. When possible, Monte Carlo results were compared to analytical models. The investigated parameters were scintillators’ detection efficiency of the incident radiation and how K-characteristic radiation affects image quality. The above scintillators were used in powder (granular) form and were examined under conditions used in general x-ray radiography, mammography, CT and nuclear medicine γ-ray imaging (γ-camera and SPECT).

1. LSO

Lutetium Oxyorthosilicate, Lu₂SiO₅ (LSO), was discovered at the beginning of the 1990’s, by Melcher and Schweitzer (Melcher and Schweitzer 1992). It has been recognized as one of the best scintillating materials. Usually, LSO is doped by Cerium activator (Ce). It has high density (7.4 g/cm³) and effective atomic number (Z_eff=66), relatively high light yield (26000 ph/MeV), suitable emission wavelength (420 nm), fast response (40ns) and it is non-hydroscopic. These properties make LSO, in single crystal form, suitable for use in γ-ray detection in nuclear medical diagnostic instruments (such as PET), high energy and nuclear physical experiments. (Melcher and Schweitzer 1992, Valais et al 2005). According to our knowledge LSO scintillator has been investigated in powder form under general radiographic and mammographic exposure conditions once experimentally (David et al 2006) and once by Monte Carlo methods (Liaparinos et al 2007). LSO scintillator has one heavy element, Lutetium (Lu, Z_Lu=71). K absorption edge energy of Lu is 63.31 keV, while Kα and Kβ characteristic radiations of Lu have energy equal to 53.07 and 54.20 keV, respectively. Therefore, LSO scintillator has increased absorption and K-characteristic effect at higher energies.
2. YSO

Yttrium Oxyorthosilicate, Y₂SiO₅ (YSO), is a scintillator which is not widely used. It can be doped by Cerium activator (Ce). It has low density (4.45 g/cm³), low light output (10000 ph/MeV), suitable emission wavelength (420 nm), short decay time (37 ns) and it is non-hygroscopic. The highest advantage of this scintillator is that Y is a cheap element, so YSO is a low cost scintillator. YSO has one heavy element, Yttrium (Y, Z₈=39). K absorption edge energy of Y is 17.04 keV, while its Kα and Kβ characteristic radiations have energy equal to 14.84 and 14.92 keV, respectively. Therefore, YSO scintillator has increased absorption and K-characteristic effect at low energies.

3. LYSO

LSO scintillator has two basic disadvantages. The first one is that Lu element is very expensive. The second one is that LSO contains a small fraction of radioactive ¹⁷⁶Lu. Therefore, LSO can be mixed with Yttrium Oxyorthosilicate, Y₂SiO₅ (YSO), creating Lutetium Yttrium Oxyorthosilicate Lu₂(1-x)Y₂xSiO₅ (LYSO). Usually, LYSO is doped by Cerium activator (Ce). It was found that LYSO has better performance and advantages compared with LSO (e.g. it has 20% higher light yield than LSO under low-energy (35 kV) x-ray excitation). Yttrium is a low cost material and it exhibits high intrinsic efficiency. Thus, LYSO is a mixed LSO/YSO non-hygrosopic crystal that offers high density (7.1 g/cm³), high light yield (30000 ph/MeV), good energy resolution (~10%) and short decay time (40 ns). These properties make LYSO ideal in a wide range of gamma ray detection applications requiring higher throughput, improved timing resolution and superior energy resolution (e.g. small animal PET).

In the present study, the performance of LYSO with concentrations varying from 90/10 up to 50/50 (ratios of LSO/YSO), was examined. LYSO scintillator has two heavy elements, Lutecium (Lu, Z₉=71) and Yttrium (Y, Z₈=39). As it was mentioned before, K absorption edge energy of Lu is 63.31 keV, while Kα characteristic radiation of Lu has energy equal to 53.07 keV and Kβ has energy equal to 54.20 keV. The corresponding K absorption edge energy of Y is 17.04 keV, while Yttrium’s Kα and Kβ characteristic radiations have energies equal to 14.84 and 14.92 keV, respectively. Therefore, LYSO has increased absorption and K-characteristic effect at both low and high energies. It may be observed that K-characteristic radiation of Lu can produce additional K-characteristic radiation to Y. This results in further degradation of the medical image quality.
4. CsI

Cesium Iodide, CsI, can be doped by both Tl and Na activators. It has intermediate density (4.51 g/cm³) and relatively high effective atomic number (Z_{eff}=52). CsI:Tl has very high light yield (66000 ph/MeV), two emission peaks at 556 and 420 nm, very long decay time (from 800 up to 6000 ns) and it is slightly hydroscopic. On the other hand, CsI:Na has high light yield (40000 ph/MeV), an emission peak at 420 nm, long decay time (63 ns) and it is hydroscopic. Both CsI:Tl and CsI:Na aren’t suitable for use in PET, because of their high decay time. Because of their hydroscopicity, they cannot be used in film-screen cassettes. They are used, usually in columnar form (needle-like crystals), in image intensifiers, Flat panels (digital radiography, radioscopy and mammography), Computed Tomography, and they are introduced in SPECT. CsI scintillator has two heavy elements, Cesium (Cs, Z_{Cs}=55) and Iodine (I, Z_{I}=53). K-absorption edge energy of Cs is 35.98 keV, while its K_{α} characteristic radiation has energy equal to 30.64 keV and K_{β} has energy equal to 30.99 keV. The corresponding K-absorption edge energy of I is 33.17 keV, while it’s K_{α} and K_{β} characteristic radiations have energies equal to 28.31 and 28.61 keV, respectively. Consequently, K-characteristic radiation of Cs cannot produce additional K-characteristic radiation to I.

5. YTaO₄

YTaO₄ is a promising material for many applications. It is usually doped by Niobium activator (Nb). It has high density (7.5 g/cm³), high light yield (40000 ph/MeV), suitable emission wavelength (410 nm), long decay time and it is non-hygroscopic. Because of its long decay time it isn’t used in PET. However, it is usually used, in granular form, in screen-film cassettes in conventional radiography. YTaO₄ has two heavy elements, Yttrium (Y, Z_{Y}=39) and Tantalum (Ta, Z_{Ta}=73). K absorption edge energy of Y is 17.04 keV, while its K_{α} and K_{β} characteristic radiations have energy equal to 14.84 and 14.92 keV, respectively. The corresponding K-absorption edge energy of Ta is 67.42 keV, while it’s K_{α} and K_{β} characteristic radiations have energy equal to 56.40 and 57.69 keV, correspondingly. Therefore, YTaO₄ scintillator has increased absorption and K-characteristic effect at both low and high energies. Just like LYSO, K-characteristic radiation of Ta can produce additional K-characteristic radiation to Y. This results in further degradation of the medical image quality.
### Table 1: Physical properties of the investigated scintillators related to the K-characteristic radiation

<table>
<thead>
<tr>
<th>Scintillator</th>
<th>( \rho ) (g/cm(^3))</th>
<th>Heavy element</th>
<th>( f_K )</th>
<th>K-edge (keV)</th>
<th>( \omega_K )</th>
<th>( K_\alpha, K_\beta ) (keV)</th>
<th>( I_\alpha/I_\beta )</th>
</tr>
</thead>
<tbody>
<tr>
<td>LSO</td>
<td>7.4</td>
<td>Lu (71)</td>
<td>0.8079</td>
<td>63.31</td>
<td>0.9487</td>
<td>53.07, 54.20</td>
<td>0.3628/0.6372</td>
</tr>
<tr>
<td>YSO</td>
<td>4.45</td>
<td>Y (39)</td>
<td>0.8542</td>
<td>17.04</td>
<td>0.7155</td>
<td>14.84, 14.92</td>
<td>0.3429/0.6571</td>
</tr>
<tr>
<td>LYSO</td>
<td>7.1</td>
<td>Lu (71)</td>
<td>0.8079</td>
<td>63.31</td>
<td>0.9487</td>
<td>53.07, 54.20</td>
<td>0.3628/0.6372</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Y (39)</td>
<td>0.8542</td>
<td>17.04</td>
<td>0.7155</td>
<td>14.84, 14.92</td>
<td>0.3429/0.6571</td>
</tr>
<tr>
<td>CsI</td>
<td>4.51</td>
<td>Cs (55)</td>
<td>0.8313</td>
<td>35.98</td>
<td>0.8942</td>
<td>30.64, 30.99</td>
<td>0.3513/0.6487</td>
</tr>
<tr>
<td></td>
<td></td>
<td>I (53)</td>
<td>0.2696</td>
<td>33.17</td>
<td>0.8819</td>
<td>28.31, 28.61</td>
<td>0.3501/0.6499</td>
</tr>
<tr>
<td>YTaO(_4)</td>
<td>7.5</td>
<td>Y (39)</td>
<td>0.8542</td>
<td>17.04</td>
<td>0.7155</td>
<td>14.84, 14.92</td>
<td>0.3429/0.6571</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Ta (73)</td>
<td>0.8048</td>
<td>67.42</td>
<td>0.9522</td>
<td>56.40, 57.69</td>
<td>0.3646/0.6354</td>
</tr>
</tbody>
</table>

As this study investigates the detection efficiency and K-characteristic effect on scintillators, Table 1 shows some relative physical properties of the scintillators. \( f_K \) is a factor expressing the relative contribution of the K-shell photoelectric cross section \( (\tau_K) \) to the total photoelectric effect cross section \( \tau \) \( (f_K = \tau_K / \tau) \). The atomic numbers of the heavy elements contained in the scintillators are shown in parenthesis in the above table.

#### B.6.5 Attenuation coefficients of scintillators

The following figures show the total mass attenuation coefficient \((\mu / \rho)_{tot,a}\) or \(\mu_T / \rho\) and photoelectric absorption coefficient \((\mu / \rho)_{\tau,a}\) or \(\mu_p / \rho\) of the investigated scintillators. \(\mu_p / \rho\) is depicted since it is used in detection efficiency calculation. It may be observed that the difference between the two coefficients is high just below K absorption edge energy and at high energies. At these energies scattering effects are more significant.
Figure 6: mass attenuation coefficients $\left(\frac{\mu}{\rho}\right)_{\text{tot},t}$ and $\left(\frac{\mu}{\rho}\right)_{\text{a},t}$ of LSO

Figure 7: mass attenuation coefficients $\left(\frac{\mu}{\rho}\right)_{\text{tot},x}$ and $\left(\frac{\mu}{\rho}\right)_{\text{a},x}$ of YSO
**Figure 8:** Mass attenuation coefficients $(\mu/\rho)_{\text{tot}}$ and $(\mu/\rho)_{\text{e}}$ of LYSO 50/50

**Figure 9:** Mass attenuation coefficients $(\mu/\rho)_{\text{tot}}$ and $(\mu/\rho)_{\text{e}}$ of LYSO 60/40
Figure 10: Mass attenuation coefficients \((\mu/\rho)_{\text{tot}}\) and \((\mu/\rho)_{\text{el}}\) of LYSO 70/30

Figure 11: Mass attenuation coefficients \((\mu/\rho)_{\text{tot}}\) and \((\mu/\rho)_{\text{el}}\) of LYSO 80/20
Figure 12: mass attenuation coefficients $\left( \frac{\mu}{\rho} \right)_{\text{tot}}$ and $\left( \frac{\mu}{\rho} \right)_{\text{e.a.}}$ of LYSO 90/10

Figure 13: mass attenuation coefficients $\left( \frac{\mu}{\rho} \right)_{\text{tot}}$ and $\left( \frac{\mu}{\rho} \right)_{\text{e.a.}}$ of CsI
B.6.6 Investigated performance of the scintillators

The performance of the above scintillators was investigated in terms of detection efficiency and K-characteristic effect. This investigation was achieved by using a custom and validated Monte Carlo simulation program dedicated to scintillators (Liaparinos et al 2006 b, Liaparinos et al 2007, Liaparinos 2007). When possible, Monte Carlo results were compared with analytical models. The detection efficiency is described by the Quantum Detection Efficiency (QDE) of the scintillators. K-characteristic effect may be described by means of (a) the number of produced K x-ray photons, (b) the number of reabsorbed K x-ray photons, (c) K-factor, (d) the probability of K-fluorescence x-ray photon generation per absorbed x-ray (PKA), (e) the probability of K-fluorescence x-ray photon generation per incident x-ray (PKI), (f) the probability of generation and reabsorption of a K-fluorescence x-ray per incident x-ray (PKR) and (g) spatial distribution of the absorbed K x-ray photons.

B.6.6.1 Quantum Detection Efficiency (QDE)

QDE expresses the fraction of incident x-ray photons detected by a phosphor screen (Yaffe and Rowlands 1997). In the present study, only photons totally absorbed within the crystal were considered in the QDE calculations. Scattered x-ray photons as well as intrinsic K-fluorescence x-rays escaping the crystal were not included in the theoretical calculations.

Figure 14: mass attenuation coefficients \( \left( \frac{\mu}{\rho} \right)_{\text{tot}} \) and \( \left( \frac{\mu}{\rho} \right)_{\text{rad}} \) of YTaO₄
Hence, this efficiency corresponds to those photons that have deposited all their energy within the scintillator. For mono-energetic radiation $QDE(E)$ may be expressed by the following equation:

$$QDE(E) = 1 - e^{-(\mu_p(E)/\rho)x}$$

(11)

where $(\mu_p(E)/\rho)$ is the x-ray mass photoelectric absorption coefficient of the scintillator, given in cm$^2$/g. $\mu_p(E)/\rho$ was calculated using tabulated data from the NIST database (Berger et al 1999). $x$ is the scintillator’s coating thickness, given in g/cm$^2$. Usually, commercial screens used in x-ray medical imaging have a thickness ranging from 10 up to 200 mg/cm$^2$ (lower values correspond to low sensitivity screens while higher values correspond to low resolution screens). As it is shown above, QDE is inversely proportional to the x-ray energy and proportional to the scintillator’s coating thickness.

### B.6.6.2 The number of produced K x-ray photons

For a given number of incident x-ray photons of constant energy, the number of K x-ray photons is expected to increase with scintillator thickness. This occurs due to the increasing probability of incident photons absorption by the scintillator. On the other hand, this number, for a given number of incident x-ray photons and constant scintillator thickness, is expected to decrease with the increase of incident x-ray photon energy. This occurs because the penetration ability of an x-ray beam is proportional to its energy. Therefore, for higher energies more x-ray photons are transmitted through the scintillator without interaction. A basic condition for K x-ray photons production is that the incident x-ray photon energy has to be higher than the K absorption edge energy of the scintillator’s high-Z element.

Additionally, the number of produced K x-ray photons is proportional to the probability of photoelectric absorption by the material, $(\mu/\rho)_{\text{r,a}}$, the relative contribution of the K-shell photoelectric cross section to the total photoelectric effect cross section, $f_K$ and the K fluorescence yield, $\omega_K$.

### B.6.6.3 The number of reabsorbed K x-ray photons

This number is proportional to the number of produced K x-ray photons. Therefore, it is proportional to the scintillator thickness and inversely proportional to the incident x-ray photon energy. Also, it is inversely proportional to the K characteristic x-ray photon energy. This
happens because when the K characteristic x-ray photon energy is high, there is an increased probability for them to escape the scintillator.

**B.6.6.4 K-factor**

K-Factor is another parameter related to the reabsorption of the K characteristic x-ray photons. It is given by the fraction of the escaped over the produced K x-ray photons. K factor’s value depends on the K characteristic x-ray photon energy and it remains unaffected by the incident x-ray photon energy. However, it depends on the scintillator thickness, because less K x-ray photons may escape from thicker scintillators.

**B.6.6.5 Probability of K-fluorescence x-ray photon generation per Absorbed x-ray (PKA)**

The probability of K-fluorescence photon production per Absorbed primary x-ray, PKA or $p_{K\tau}$, may be given as (Chan and Doi 1983 a, Kandarakis et al 2003, Kandarakis et al 2005, Kandarakis et al 2006):

$$p_{K\tau}(E) = \frac{w_Z}{\rho} \frac{\mu_p(Z,E)/\rho}{\mu_t(E)/\rho} f_K \omega_K I_y$$

where $w_Z$ is the fractional weight of the higher atomic number (Z) element in the scintillator (i.e. Lu, Y, Cs, I and Ta in the investigated scintillators), which exhibits the higher probability for photoelectric interaction. $\mu_p(Z,E)/\rho$ is the total mass photoelectric x-ray attenuation coefficient of the high-Z element at energy E. $\mu_t(E)/\rho$ is the total x-ray mass attenuation coefficient of the scintillator material at energy E. $f_K$ is the factor expressing the relative contribution of the K-shell photoelectric cross section ($\tau_K$) to the total photoelectric effect cross section $\tau_0$ ($f_K = \tau_K/\tau_0$). $\omega_K$ is the K-fluorescence yield of the higher atomic number (Z) element within the scintillator. $I_y$ is the relative frequency of either K_a or K_b fluorescence x-ray photon production. The index y stands either for a K_a or a K_b x-ray fluorescence photon. (Chan and Doi 1983 a). The nominator and the denominator of the fraction, i.e. the ratio containing the photon interaction coefficients and the fractional weight express the probability for photoelectric interaction with the high-Z element.
B.6.6.6 Probability of K-fluorescence x-ray photon generation per Incident x-ray (PKI)

The scintillator was assumed to be divided into a large number (I) of elementary thin layers of thickness $\Delta L$. The probability, $p_{Fy}^i$, of generating a K-fluorescence photon in the $i^{th}$ layer of the scintillator, after the incidence of a radiation photon of energy $E$, may be written as follows (Chan and Doi 1983 a, Kandarakis et al 2003, Kandarakis et al 2005, Kandarakis et al 2006):

$$p_{Fy}^i(E) = PKA(E) \times \left\{ \exp \left[ -\frac{\mu_r(E)}{\rho} (t-1)\Delta L \right] - \exp \left[ -\frac{\mu_r(E)}{\rho} t\Delta L \right] \right\} \quad (13)$$

The factor in curly brackets gives the attenuation of incident radiation within the $i^{th}$ layer. Then the probability, PKI or $p_{Fy}^L$, of generating a K-characteristic fluorescence photon within the whole scintillator per incident primary x-ray photon may be calculated by sum:

$$p_{Fy}^L(E, E) = \sum_{i=1}^{I} p_{Fy}^i(E) \quad (14)$$

B.6.6.7 Probability of generation and Reabsorption of a K x-ray per incident x-ray (PKR)

The following figure is essential for the understanding of the probability of generation and reabsorption of a K x-ray per incident x-ray:

![Geometrical configuration for calculating K-fluorescence emission](Figure 15: Geometrical configuration for calculating K-fluorescence emission)
The probability of a K-fluorescence x-ray photon, generated at the $i^{th}$ scintillator layer, emitted within a solid-angle element $\Delta\Omega_j$, and interacting at the $e^{th}$ layer, may be written by the following equation (Chan and Doi 1983 a, Kandarakis et al 2003, Kandarakis et al 2005, Kandarakis et al 2006):

$$p_{A,j}^{i,e}(E_y, \Delta\Omega_j) = \frac{\Delta\Omega_j}{4\pi} \left\{ \exp \left[ -\frac{\mu_t(E_y) / \rho(\left| e-i \right|-1)\Delta L}{\cos(j\Delta z)} \right] \right. $$

$$- \exp \left[ -\frac{\mu_t(E_y) / \rho(\left| e-i \right|)\Delta L}{\cos(j\Delta z)} \right] \right\} \tag{15}$$

where the solid-angle element $\Delta\Omega_j$ is calculated as follows (Chan and Doi 1983 a, Kandarakis et al 2003):

$$\Delta\Omega_j = \int_{(j-1)\Delta z}^{j\Delta z} \frac{2\pi r^2 \sin\phi d\phi}{r^2} = 2\pi \left\{ \cos(j\Delta z) - \cos j\Delta z \right\} \tag{16}$$

where $\phi$ denotes the semi-angle of the cone subtended at the point of K-characteristic x-ray fluorescence emission (see Figure 15), $\Delta\xi_j$ is the polar angle element corresponding to the solid-angle element $\Delta\Omega_j$, and $r$ is the radius of a sphere centred at the point of emission. The factor in curly brackets in relation (15) expresses the interaction of K-fluorescence photons within the $e^{th}$ layer.

The probability, PKR or $p_{A,F}^L$, of generation and absorption of a K-fluorescence photon within the whole scintillator, is obtained after summation over all the elementary thin layers $i$ and $e$ and over the solid angle elements $j$, as follows:

$$p_{A,F}^L(E_y) = \sum_{i=1}^{I} p_{Fy}^i(E_y, E_y) \sum_{j=1}^{J} \sum_{e=1}^{E} p_{A,j}^{i,e}(E_y, \Delta\Omega_j) \tag{17}$$

Equation (15) is used for scintillators with one high-Z element. For two high-Z element scintillators, the calculation of PKR using analytical model becomes more complicated (Chan and Doi 1983 a) and it is out of the present investigation’s interest. Therefore, the calculation of PKR for two high-Z element scintillators was carried out only via Monte Carlo methods.
B.6.6.8 Spatial distribution of the absorbed K x-ray photons (number and energy)

This parameter denotes the distribution of the K x-ray photons interacting within through photoelectric effect and depositing the total energy to the scintillator. As it was mentioned before, K-fluorescence photons may be emitted isotropically to all directions. Therefore, they may be absorbed to all directions. The absorption probability depends on scintillator thickness and K x-ray photon energy (Boone et al 1999).
CHAPTER C

MONTE CARLO METHODS

C.1 Introduction ................................................................. 42
C.2 Sampling techniques ..................................................... 44
  C.2.1 Inverse method ...................................................... 44
  C.2.2 Acceptance-Rejection method ................................... 45
C.1 Introduction

Numerical methods, known as Monte Carlo methods, can be described as statistical simulation methods, where statistical simulation is defined in quite general terms to be any method that utilizes sequences of random numbers to perform the simulation. Monte Carlo methods have been used for centuries, but only in the past several decades has the technique gained the status of a full-fledged numerical method capable of addressing the most complex applications. The name “Monte Carlo” was coined by Metropolis (inspired by Ulam's interest in poker) during the Manhattan Project of World War II, because of the similarity of statistical simulation to games of chance, and because the capital of Monaco was a center for gambling and similar pursuits. Monte Carlo is now used routinely in many diverse fields, from the simulation of complex physical phenomena such as radiation transport in the earth's atmosphere and the simulation of the esoteric subnuclear processes in high energy physics experiments, to the simulation of games of chance. The analogy of Monte Carlo methods to games of chance is a good one, but the “game” is a physical system, and the outcome of the game is not a pot of money or stack of chips (unless simulated) but rather a solution to some problem. The “winner” is the scientist, who judges the value of his results on their intrinsic worth, rather than the extrinsic worth of his holdings.

Statistical simulation methods may be contrasted to conventional numerical discretization methods, which typically are applied to ordinary or partial differential equations that describe some underlying physical or mathematical system. In many applications of Monte Carlo, the physical process is simulated directly, and there is no need to even write down the differential equations that describe the behaviour of the system. The only requirement is that the physical (or mathematical) system be described by probability density (or distribution) functions (pdf's). Once the pdf's are known, the Monte Carlo simulation can proceed by random sampling from the pdf's. Many simulations are then performed (multiple “trials” or “histories”) and the desired result is taken as an average over the number of observations (which may be a single observation or perhaps millions of observations). In many practical applications, one can predict the statistical error (the “variance”) in this average result, and hence an estimate of the number of Monte Carlo trials that are needed to achieve a given error.

Figure 16 illustrates the idea of Monte Carlo, or statistical simulation as applied to an arbitrary physical system. Assuming that the evolution of the physical system can be described by probability density functions (pdf's), then the Monte Carlo simulation can proceed by
sampling from these pdf's, which necessitates a fast and effective way to generate random numbers uniformly distributed on the interval \((0,1]\). The outcomes of these random samplings, or trials, must be accumulated or tallied in an appropriate manner to produce the desired result, but the essential characteristic of Monte Carlo is the use of random sampling techniques (and perhaps other algebra to manipulate the outcomes) to arrive at a solution of the physical problem. In contrast, a conventional numerical solution approach would start with the mathematical model of the physical system, discretizing the differential equations and then solving a set of algebraic equations for the unknown state of the system.

![Monte Carlo simulation of physical system](image)

**Figure 16:** Monte Carlo simulation of physical system

Some of the applications of Monte Carlo simulation are in the following fields: nuclear reactors design, quantum chromodynamics, radiation cancer therapy, traffic flow, econometrics, VLSI design and medical imaging.

The Monte Carlo technique of radiation transport consists of using knowledge of pdf’s governing the individual interactions of electrons and photons to simulate their transport through matter. The resultant distributions of physical quantities of interest from a large number of simulated particles (called “histories”), provides a description on the average transport properties and the associated distributions. Since the Monte Carlo method uses well-established physics principles describing the nature of the interactions, the technique assures accurate results if the code is implemented correctly and enough histories are run.
C.2 Sampling techniques

In this section some procedures are taken into consideration for generating *random* variables from different distributions. Two sampling techniques were considered in the present study: (a) Inverse method and (b) Acceptance-rejection method.

C.2.1 Inverse method

Variable $X$ is considered to be a random variable with cumulative distribution function (cdf) $F_X(x)$. To get a value, say $x$, of a random variable $X$, obtain a value, say $u$, of a random variable $U$, compute $F_X^{-1}(u)$, and set it equal to $x$ (Figure 17).

![Diagram of the Inverse method](image)

Figure 17: Inverse method

More specific the algorithm of the inversion technique can be described with the following steps (Rubenstein 1981):

1. Consider $f(x)$ a pdf, $x \in [a, b]$

2. Check if $f(x)$ is normalized: $\int_a^b f(x) \, dx = 1$

3. Calculate the cdf: $F(x) = \int_a^x f(x) \, dx$

4. Generate random number $R$

5. Let $F(x) = R$ and solve for $x$: $x = F^{-1}(R)$
C.2.2 Acceptance-Rejection method

This method consists of sampling a random variable from an appropriate distribution and subjecting it to a test in order to determine whether or not it will be acceptable for use. Consider \([a, b]\) the allowed range of values of the variable \(x\), and \(p_{\text{max}}\) the maximum of the density \(p(x)\) (see Figure 18).

![Figure 18: Acceptance-Rejection method](image)

The algorithm of the acceptance-rejection method may be described with the following steps:

1. Consider \(f(x)\) a pdf, \(x \in [a, b]\)
2. Set \(g(x) = \frac{f(x)}{p_{\text{max}}}\).
3. Generate a random number \(R_1 \in [0, 1)\).
4. Generate a random value of \(x \in [a, b]\), say \(x^* = a + (b - a)R_1\).
5. Generate a random number \(R_2 \in [0, 1)\).
6. Compare \(R_2\) with \(g(x^*)\):
   
   If \(g(x^*) \leq R_2\) then Reject \(x^*\), otherwise Reject \(x^*\). Return to the fourth step.
CHAPTER D

MATERIALS AND METHODS-THE MONTE CARLO MODEL

D.1 Geometry of the simulation .................................................................47
D.2 Simulation of the x-ray photon history inside the scintillator ........47
  D.2.1 Photoelectric absorption .............................................................48
  D.2.2 Compton scattering .................................................................49
  D.2.3 Rayleigh scattering .................................................................49
D.3 Input data required to the Monte Carlo program .......................50
D.4 Calculated output parameters by the Monte Carlo program ........50
D.5 Average absolute relative difference between Monte Carlo and theoretical values .................................................................51
D.1 Geometry of the simulation

The phosphor screen was modeled as a three-dimensional layer consisting of uniformly distributed grains. All grains were of the same size (7μm), which was considered to be equal to the average size of the grains contained in a commercial screen. The phosphor screen (layer) thickness was varying from 20 up to 100 mg/cm². The screen area (surface dimensions) was considered to be 5x5 cm² in all cases except for the spatial distribution of K x-ray photons case (5x5 mm²). The screen packing density, \( p_p \), was equal to 0.5 (50%). Monoenergetic incident x-ray photons were assumed, having energy in the range from 20 up to 160 keV. Energies from 20 up to 80 keV were used for simulation of conditions used in x-ray mammography, in general x-ray radiography and in CT. This energy range was selected by calculating the mean energies corresponding to two limiting cases of x-ray imaging (e.g. x-ray mammography and CT). For instance, the mean energy at 30 kVp for Mo/0.030mmMo anode/filter material combination, plus 30 mm of Lucite (for human breast simulation), was found 19.41 keV (Boone et al 1997, Boone 1998). The respective mean energy of a 140 kVp beam with W/2mmAl anode/filter material combination, plus 20 mm of Aluminum (for human body simulation), was found 74.28 keV (Boone and Seibert 1997, Boone 1998). Higher energies were also considered to simulate nuclear medicine \( \gamma \)-ray imaging conditions (e.g. \(^{99m}\)Tc at 140 keV and \(^{201}\)Tl etc). In order to minimize the statistical fluctuation of the results, the number of x-ray photons in all studies was \( 10^6 \). Incident x-ray photons were assumed to impinge on the screen surface according to narrow beam geometry. Applying \( 10^6 \) monoenergetic x-ray photons, the required computation time for each simulation of the aforementioned phosphor materials was varying from 17 up to 162 minutes, using a single-processor P4 with 2.40 GHz and 1024 MB access memory. The broad range in computation time depends on the fraction of incident x-rays which were absorbed by the scintillator.

D.2 Simulation of the x-ray photon history inside the scintillator

The x-ray photon history, used in this study, was simulated using a custom and validated Monte Carlo simulation program, dedicated to scintillators and developed in MATLAB (Liaparinos et al 2006 b, Liaparinos et al 2007, Liaparinos 2007). This software was differentiated from its initial version 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 (i.e. LYSO, CsI and YTaO₄).
An x-ray photon history was considered to start when the x-ray photon, with energy having a single value (monoenergetic beam), impinged on the phosphor screen surface. The coordinates of the initial position and the initial direction angles (polar and azimuthal) of the x-ray photon were determined according to the considered beam geometry (narrow beam). A reference coordinate system was employed, whose origin was located at the edge of phosphor screen. For each x-ray energy value \( E \), the total mass attenuation coefficient, the mass attenuation coefficients corresponding to each one of the x-ray interactions (Photoelectric, Compton and Rayleigh effects) and the mass attenuation coefficient for each element of the phosphor (e.g. \( (\mu/\rho)_{\text{Cs}} \) and \( (\mu/\rho)_{\text{I}} \) in CsI) were determined using logarithmic interpolation on the corresponding stored tabulated data. These data were obtained using the XCOM software, which is a photon cross section database of the National Institute of Standards and Technology (NIST) (Berger et al. 1999). The x-ray photon was considered to penetrate the screen and its transport through the phosphor slab was described in terms of the mean photon free path length (fpl) and the interaction site coordinates. If the free path length brings the interaction site coordinates outside the scintillator, the incident x-ray photon is considered to escape. In this case, it interacts with the scintillator material. The three most possible interactions for the investigated energies (up to 160 keV) are the Photoelectric absorption, Compton (incoherent) scattering and Rayleigh (coherent) scattering.

D.2.1 Photoelectric absorption

If the incident x-ray photon undergoes photoelectric absorption, a sequence of processes may occur depending on its energy \( E \) (Liaparinos et al 2006 b). When the photon energy is larger than the K-shell binding energy, \( E_K \), photoelectric absorption may occur either in the K-shell or in the L-shell. In the case of the K-shell, the emission of K-characteristic radiation or the production of Auger electrons depends on the K-fluorescence yield \( \omega_K \). In the case of K-characteristic radiation, a new x-ray photon is produced, whose trajectory within the phosphor screen is examined separately. Otherwise, an Auger electron is emitted, which is assumed to be locally absorbed. In the present study, the two following K-fluorescence emission processes were considered: K-L2 (K\( \alpha \)) and K-L3 (K\( \beta \)) radiative transitions and the K-L-X Auger transitions, where X denotes a shell with negligible binding energy. The energy of the K-fluorescence photon or the energy deposited in the phosphor by an Auger electron was determined according to the corresponding probability of each possible transition.
The coordinates of the K x-ray photon produced were determined from the coordinates of the interaction site of the initial x-ray photon. It was assumed that the K-characteristic photons were emitted in any direction, following an isotropic distribution. The polar angle $\theta$ and the azimuthal angle $\phi$ of the emission’s distribution were sampled according to the respective cdf (Liaparinos et al 2006 b). In the case that they do not escape the scintillator, they may interact with it through the three basic interactions. If they interact through Photoelectric absorption, they are considered to be absorbed by the scintillator material. For two high-Z element scintillators, the K x-ray photons of the high-Z element may be absorbed by the low-Z element resulting in the Additional K-characteristic radiation production. These photons can in turn interact with the scintillator material through the three basic interactions.

Finally, the initial x-ray photon was assumed to be locally absorbed when: (a) the x-ray photon energy was larger than the K-shell binding energy $E_K$ and at the same time the photoelectric effect occurred in the L-shell, (b) the x-ray photon energy was smaller than the $E_K$ but larger than the average L-shell binding energy $E_L$ and (c) the x-ray photon energy was smaller than 5 keV (cut off energy) (Morin 1988).

**D.2.2 Compton scattering**

In this case, the incident x-ray photon undergoes incoherent (Compton) scattering through collision with a loosely bound atomic electron. As a result, it transfers some of its energy and momentum to the electron (recoil electron) and it is deflected by shaping an angle $\theta$ with respect to its original direction. The recoil electron was assumed to be locally absorbed and the scattered photon was assumed to be transported within phosphor material having a new direction and energy. The new direction of the scattered photon is described by the polar angle $\theta$ and the azimuthal angle $\phi$, in a coordinate system that has its origin at the interaction site and its z-axis along the initial photon direction. The azimuthal angle $\phi$ of the scattered photon was sampled randomly in the interval $[0,\pi]$. The polar angle $\theta$ was sampled from the differential cross section for incoherent scattering, using the sampling algorithm described by Brusa et al (1996).

**D.2.3 Rayleigh scattering**

If the incident x-ray photon undergoes coherent (Rayleigh) scattering, the scattered photon acquires new direction without depositing any energy within the phosphor screen. The new direction of the scattered photon is described by the polar angle $\theta$ and the azimuthal angle $\phi$. 
The coordinate system was considered to have its origin at the interaction site and its z-axis along the initial photon direction. The azimuthal angle $\phi$ of the scattered photon was sampled randomly in the interval $[0,2\pi)$. The polar angle $\theta$ was sampled from the differential cross section for coherent scattering, which was described by Morin (1988) and Chan and Doi (1983 b).

**D.3 Input data required to the Monte Carlo program**

The initial custom and validated Monte Carlo simulation program investigates almost all the processes inside the scintillator, from the incidence of the x-ray photons to the scintillator, to the exit of the light photons from it. However, the present study focuses on the absorption efficiency and K-characteristic effect. Therefore, numerical values of various physical parameters and coefficients relevant to x-ray interactions through the material were required. All values were taken from validated tabulated data and libraries. More specifically, the employed parameters and coefficients were the following:

Data relevant to the mass attenuation coefficients of the material (Berger et al 1999), the mass partial interaction coefficients of the material (Berger et al 1999), the mass partial interaction coefficients of each element of the chemical compound and their fractional weight (Berger et al 1999), the incoherent scattering functions (Hubbell et al 1975), the atomic form factors (Hubbell et al 1975), the probability of the K or L-shell contribution to the photoelectric effect (Cullen et al 1997, Boone and Chavez 1996), the K-fluorescence yield (Hubell et al 1994) for the production of characteristic radiation or the probability of Auger electron production, the K or L shell binding energies (Cullen et al 1997) and the transition probabilities of atom relaxation (Cullen et al 1997).

**D.4 Calculated output parameters by the Monte Carlo program**

From the previously described Monte Carlo simulation, numerical evaluations concerning the x-ray photon absorption or escape events were carried out. Furthermore, for every (incident or K characteristic) x-ray interaction and absorption event, information on the deposited amount of the x-ray energy and its spatial distribution was obtained. These evaluations and the corresponding information were used in the assessment of the following phosphor screen parameters:

(i) The Quantum Detection Efficiency (QDE). It is the fraction of the number of absorbed x-ray photons over the incident x-ray photons. An x-ray photon was considered to be
absorbed, only after Photoelectric absorption event occurred, resulting in totally energy deposition to the material. For example, if an incident x-ray photon makes three consecutive Compton scattering events and finally escapes the scintillator, it is regarded as an escaped x-ray photon.

(ii) The number of produced K x-ray photons. It was calculated through a counter which increased every time that a K x-ray production took place.

(iii) The number of reabsorbed K x-ray photons. This parameter counts the number of K x-ray photons that have interacted through Photoelectric effect with the material and deposited their whole energy to it.

(iv) The K-Factor is the fraction of the escaped over the produced K x-ray photons.

(v) The Probability of K-fluorescence x-ray photon generation per Absorbed x-ray (PKA). PKA is the fraction of produced K x-ray photons over the absorbed x-ray photons.

(vi) The Probability of K-fluorescence x-ray photon generation per Incident x-ray (PKI). It is the fraction of produced K x-ray photons over the incident x-ray photons.

(vii) The Probability of generation and Reabsorption of a K x-ray per incident x-ray (PKR). PKR was calculated by the fraction of reabsorbed K x-ray photons over the incident x-ray photons.

(viii) The Spatial distribution of the absorbed K x-ray photons (number and energy). The scintillator slab was partitioned into 50 small areas. The central area had dimensions equal to 100x100 μm². Each of the rest 49 areas had sides 100 μm larger than the previous one. Therefore, the last area had dimensions 5x5 mm². The number of the K x-ray photons absorbed within each area was calculated. Additionally, the respective absorbed energy within each area was evaluated. The absorbed energy’s evaluation was made by the addition of the number of absorbed K x-ray photons of a specific element times their energy. For example, for LYSO scintillator the absorbed energy of K photons at a specific area was given by the number of absorbed K photons of Lu times their energy (~53.79 keV) plus the absorbed K photons of Y times their energy (~14.89 keV).

D.5 Average absolute relative difference between Monte Carlo and theoretical values

The absolute relative difference between values obtained by Monte Carlo (MC) and the corresponding theoretical values (TH) may be given by the following formula:
The average absolute relative difference is the average value of the aforementioned parameter. The latter indicates how relative the Monte Carlo and theoretical models are for a specific input or output parameter, under the same or relevant conditions.

\[
\frac{|MC - TH|}{TH} \cdot 100 \, \% 
\]
CHAPTER E

RESULTS AND DISCUSSION

E.1 Quantum Detection Efficiency (QDE) ................................................................. 54
E.2 The number of produced and absorbed K x-ray photons ......................... 62
E.3 K-Factor .............................................................................................................. 74
E.4 Probabilities for K x-ray photons (PKA, PKI and PKR) ......................... 80
E.5 Spatial distribution of the absorbed K x-ray photons (number and energy) ........................................................................................................ 88
E.1 Quantum Detection Efficiency (QDE)

The quantum detection efficiency of LSO phosphor with respect to the incident x-ray energy (keV) is shown in Figure 19. In this figure Monte Carlo results are compared with theoretical model obtained by equation (11), in the energy range from 5 up to 160 keV. The presented data were calculated for three coating thicknesses of phosphor screen, suggested for use in mammography (34 mg/cm²) and x-ray radiography (60 and 100 mg/cm²) respectively. The dots correspond to values obtained by Monte Carlo, while the curve represents the theoretical model.

![Figure 19. QDE versus x-ray energy for 34, 60 and 100 mg/cm² of LSO scintillator calculated by Monte Carlo methods (MC) and validated by theoretical curves (TH).](image)

It may be observed that QDE is decreasing with increasing x-ray energy, because x-ray photons become more penetrating and they interact less with the scintillator. The sudden increase of QDE values at certain energy (63.3 keV) corresponds to the influence of photoelectric K-absorption edge of Lu (i.e. there is a high probability for incident x-rays to be absorbed by the scintillator). The absolute relative differences between Monte Carlo and theoretical calculations were 0.73 %, 1.02 % and 1.29 % for 34, 60 and 100 mg/cm², respectively. These differences were due to the limitations of the theoretical approximation (Equation (11)), which does not take into consideration the scatter effect. An incident photon can interact through coherent or incoherent scatter with scintillator and then be absorbed through photoelectric effect.
Figure 20 illustrates QDE variation with regard to screen coating thickness for LSO scintillator and four constant x-ray energies (20, 65, 80 and 140 keV). QDE values are increasing with increasing coating thickness. This occurs due to the higher probability of interaction between x-ray photons and the phosphor screen. The absolute relative differences between Monte Carlo and theoretical calculations varied from 0.20 up to 1.44 %.

![Figure 20](image)

**Figure 20.** QDE versus screen coating thickness for LSO phosphor and four x-ray energies (20, 65, 80 and 140 keV), calculated by Monte Carlo methods (MC) and validated by theoretical curves (TH).

Figure 21 presents the variation of QDE with x-ray energy in the range from 5 up to 160 keV, for three coating thicknesses (34, 60 and 100 mg/cm\(^2\)) of YSO scintillator. This figure indicates the effect of K-absorption edge of Y at 17.04 keV. The absolute relative differences between Monte Carlo and theoretical calculations varied from 1.36 up to 2.27 %.

![Figure 21](image)

**Figure 21.** QDE versus x-ray energy for 34, 60 and 100 mg/cm\(^2\) of YSO scintillator calculated by Monte Carlo methods (MC) and validated by theoretical curves (TH).
Figure 22 shows QDE variation versus screen coating thickness for YSO scintillator and four constant x-ray energies (20, 40, 80 and 140 keV). The absolute relative differences between Monte Carlo and theoretical calculations varied from 0.12 up to 2.51 %.

![Figure 22. QDE versus screen coating thickness for YSO phosphor and four x-ray energies (20, 40, 80 and 140 keV), calculated by Monte Carlo methods (MC) and validated by theoretical curves (TH).](image1)

The variation of QDE with regard to x-ray energy in the range from 5 up to 160 keV, for three coating thicknesses (34, 60 and 100 mg/cm$^2$) of LYSO 50/50 scintillator, is depicted in Figure 23. The absolute relative differences between Monte Carlo and theoretical calculations varied from 0.68 up to 1.41 %. This figure shows the effects of K-absorption edges of both Y and Lu at 17.04 and 63.31 keV respectively.

![Figure 23. QDE versus x-ray energy for 34, 60 and 100 mg/cm$^2$ of LYSO 50/50 scintillator calculated by Monte Carlo methods (MC) and validated by theoretical curves (TH).](image2)
The variation of QDE versus screen coating thickness for LYSO 50/50 scintillator and four constant x-ray energies (20, 65, 80 and 140 keV) is shown in Figure 24. The absolute relative differences between MC and theoretical calculations were found to vary from 0.17 up to 1.5 %.

![Figure 24. QDE vs screen coating thickness for LYSO 50/50 phosphor and four x-ray energies (20, 65, 80 and 140 keV), calculated by Monte Carlo methods (MC) and validated by theoretical curves (TH).](image)

For brevity reasons, the calculated QDE values corresponding to LYSO 60/40, LYSO 70/30 and LYSO 80/20 are not depicted. However, a comparison between all ratios of LSO/YSO is depicted in the following figures. Figure 25 shows the variation of QDE with x-ray energy in the range from 5 up to 160 keV, for three coating thicknesses (34, 60 and 100 mg/cm²) of LYSO 90/10 scintillator. The absolute relative differences between Monte Carlo and theoretical calculations were varied 0.61 up to 1.03 %.

![Figure 25. QDE versus x-ray energy for 34, 60 and 100 mg/cm² of LYSO 90/10 scintillator calculated by Monte Carlo methods (MC) and validated by theoretical curves (TH).](image)
Figure 26 shows QDE variation with screen coating thickness for LYSO 90/10 scintillator and four constant x-ray energies (20, 65, 80 and 140 keV). The absolute relative differences between Monte Carlo and theoretical calculations varied from 0.19 up to 2.45 %.

Figure 26. QDE vs screen coating thickness for LYSO 90/10 phosphor and four x-ray energies (20, 65, 80 and 140 keV), calculated by Monte Carlo methods (MC) and validated by theoretical curves (TH).

Figure 27 illustrates a comparison of QDE values corresponding to LYSO 50/50 and LYSO 90/10 under the same conditions (coating thickness equal to 100 mg/cm² in the energy range from 5 up to 160 keV).

Figure 27. Comparison of LYSO 50/50 and the LYSO 90/10 for the QDE of the same coating thickness (100 mg/cm²), calculated by Monte Carlo methods (MC) and validated by theoretical curves (TH).
It was found that the QDE of the two scintillators had almost the same value in the energy range from the K-edge of Y (17.04 keV) up to the K-edge of Lu (63.31 keV). For higher energies, LYSO 90/10 had higher absorption efficiency than that of LYSO 50/50. This happens due to the photoelectric K-absorption edge of Lu, i.e. there is a higher probability for incident x-rays to be absorbed by the scintillator. This effect has higher impact on the LYSO 90/10 than on LYSO 50/50 scintillator, because the first one has higher fraction of Lu. The average differences between Monte Carlo and theoretical calculations were 1.41 % and 0.83 % for LYSO 50/50 and LYSO 90/10 scintillators, respectively.

Figure 28 shows QDE variation versus screen coating thickness for all scintillators of the same x-ray energy (65 keV). It may be observed that for the same coating thickness, detection efficiency is increasing with the increase of the Lu fraction inside the LYSO scintillator. This happens because Lu (Z_{Lu}=71) is a heavier element than Y (Z_{Y}=39). Therefore, it increases the photoelectric absorption probability.

The variation of QDE with x-ray energy in the range from 5 up to 160 keV, for three coating thicknesses (34, 60 and 100 mg/cm^2) of CsI scintillator is illustrated in Figure 29. The absolute relative differences between Monte Carlo and theoretical calculations varied from 0.66 up to 1.33 %. This figure shows the effects of K-absorption edges of both Cs and I at 35.98 and 33.17 keV, respectively. The effect of the K-absorption edge of Cs is more significant than that of I.
The variation of QDE with regard to screen coating thickness for CsI scintillator and four constant x-ray energies (20, 40, 65 and 140 keV) is shown in Figure 30. The absolute relative differences between MC and theoretical calculations were found to vary from 0.22 up to 1.5 %.

Figure 31 shows the variation of QDE with x-ray energy in the range from 5 up to 160 keV, for three coating thicknesses (34, 60 and 100 mg/cm²) of YTaO₄ scintillator. This figure shows the effects of K-absorption edges of both Y and Ta at 17.04 and 67.42 keV, respectively. The absolute relative differences between Monte Carlo and theoretical calculations ranged from 0.75 up to 1.32 %.
Figure 31. QDE versus x-ray energy for 34, 60 and 100 mg/cm² of YTaO₄ scintillator calculated by Monte Carlo methods (MC) and validated by theoretical curves (TH).

Figure 32 depicts QDE variation versus screen coating thickness for YTaO₄ scintillator and four constant x-ray energies (20, 40, 70 and 140 keV). The absolute relative differences between Monte Carlo and theoretical calculations varied from 0.14 up to 1.32 %.

Finally, Figure 33 shows the comparative detection efficiencies of all the above scintillators for the same coating thickness (60 mg/cm²) and energy ranging from 5 up to 160 keV.
LSO scintillator has slightly higher detection efficiency values than that of LYSO 90/10 for energies above the K-absorption edge energy of Lu (63.31 keV). On the other hand, LYSO 50/50 scintillator has much lower values than LSO for energies above 63.31 keV. YSO has almost the same QDE values as the aforementioned scintillators in the energy range from the K-absorption edge of Y (17.03 keV) up to the K-absorption edge of Lu. After 63.31 keV YSO has very low QDE values, due to the lack of Lu element. YTaO₄ scintillator has slightly higher QDE values than the previous scintillators for energies up to 63.31 keV. After K-absorption edge energy of Ta (67.42 keV) it has values similar to those of LYSO 70/30. Finally, CsI scintillator has high values at lower energies (the K-absorption edge of Cs is at 35.98 keV). However, it may be observed that for energies above 63.31 keV it has almost the same values as LYSO 50/50.

E.2 The number of produced and absorbed K x-ray photons

Figure 34 shows the variation of the number of incident and absorbed x-ray photons with x-ray energy for a particular coating thickness (34 mg/cm²) of LSO scintillator. Also, it depicts the variations of the number of produced and absorbed K x-ray photons of Lu. The produced and absorbed K x-ray photons of Lu exist for energies above the K-absorption edge energy of Lu (63.31 keV). It may be observed that the number of both the produced and absorbed K x-ray photons decreases with the increase of x-ray energy. This happens because the incident x-ray photons become more penetrating and they interact less with the scintillator.
Figure 34. Number of incident, absorbed x-ray, produced and absorbed K-fluorescence x-ray photons versus x-ray energy for 34 mg/cm² of LSO, calculated by Monte Carlo.

Figure 35 illustrates variations of the parameters shown in Figure 34. The difference in this case, is that the variations are proportional to the coating thickness of LSO scintillator, for a constant incident x-ray photon energy (65 keV). The latter has selected to have value close to K-absorption edge energy of Lu (63.31 keV), so the K characteristic radiation effect is more important. The number of both produced and absorbed K x-ray photons increases as a function of phosphor coating thickness, because of the increased number of the absorbed x-ray photons.

Figure 35. Number of incident, absorbed x-ray, produced and absorbed K-fluorescence x-ray photons versus coating thickness of LSO and for constant x-ray energy (65 keV), calculated by Monte Carlo.

Figure 36 depicts the variation of the number of incident and absorbed x-ray photons with x-ray energy for a particular coating thickness (34 mg/cm²) of YSO scintillator. Also, it depicts
the variations of the number of produced and absorbed K x-ray photons of Y. The produced and absorbed K x-ray photons of Y exist for energies above the K-edge energy of Y (17.04 keV).

![Graph showing variations](image)

**Figure 36.** Number of incident, absorbed x-ray, produced and absorbed K-fluorescence x-ray photons versus x-ray energy for 34 mg/cm² of YSO, calculated by Monte Carlo.

Figure 37 shows the same parameters presented in Figure 36, proportional to YSO scintillator’s coating thickness for a constant incident x-ray photon energy (20 keV).

![Graph showing variations](image)

**Figure 37.** Number of incident, absorbed x-ray, produced and absorbed K-fluorescence x-ray photons versus coating thickness of YSO and for constant x-ray energy (20 keV), calculated by Monte Carlo.

Figure 38 shows the variation of the number of incident and absorbed x-ray photons with x-ray energy for a particular coating thickness (34 mg/cm²) of LYSO 50/50 scintillator. Also, it depicts the variations of the number of produced K x-ray photons of Lu (K_Lu), the K x-ray
photons of Y because of incident x-ray photons (K\textsubscript{Y}/inc) and the K-photons of Y because of the produced K x-ray photons of Lu (K\textsubscript{Y}/Lu). Finally, it presents the total number of produced K x-ray photons of Y (K\textsubscript{Y} = K\textsubscript{Y}/inc + K\textsubscript{Y}/Lu) in the energy range from 20 up to 160 keV. For the same x-ray energy the number of produced K x-ray photons of Lu is higher than the respective number of Y. This can be explained by the fact that Lu is heavier than Y, so it has a higher total mass attenuation coefficient for a specific energy. Therefore, it may absorb a larger number of incident x-ray photons, which in turn can produce K x-ray photons. Also, for the same parameters the number of K\textsubscript{Y}/inc is higher than that of K\textsubscript{Y}/Lu. This happens because the number of incident x-ray photons is higher than the number of K x-rays produced by Lu. However, the K\textsubscript{Y}/Lu increase rapidly with coating thickness, due to the increase of the production of K x-rays of Lu and their reabsorption by Y element (see Figure 40 and 41).

![Figure 38](image1.png)

**Figure 38.** Number of incident, absorbed x-ray and produced K-fluorescence x-ray photons versus x-ray energy for 34 mg/cm\(^2\) of LYSO 50/50, calculated by Monte Carlo.

Figure 39 illustrates the corresponding absorbed K x-ray photons for the parameters investigated in Figure 38. It may be observed that the number of absorbed K x-ray photons of Y element is slightly lower than that of Lu, despite the big difference between the two elements in the production of K x-ray photons. This happens because the produced K x-ray photons of Lu have higher average energy (53.79 keV) than that of Y element (14.89 keV), consequently they have higher tendency to escape the scintillator.
Figure 39. Number of absorbed x-ray and absorbed K-fluorescence x-ray photons versus x-ray energy for 34 mg/cm² of LYSO 50/50, calculated by Monte Carlo.

Figure 40 depicts variations of the parameters shown in Figure 38. The difference in this case, is that the variations are proportional to the coating thickness of LYSO 50/50 scintillator, for a constant incident x-ray photon energy (65 keV).

Figure 41 shows the same parameters depicted in Figure 39, proportional to LYSO 50/50 scintillator’s coating thickness for a constant incident x-ray photon energy (65 keV).
Figure 41. Number of absorbed x-ray and absorbed K-fluorescence x-ray photons versus coating thickness of LYSO 50/50 and for constant x-ray energy (65 keV), calculated by Monte Carlo.

For brevity reasons, the calculated numbers of produced and absorbed K x-ray photons corresponding to LYSO 60/40, LYSO 70/30 and LYSO 80/20 are not depicted. However, the respective numbers of parameters shown for LYSO 50/50 are shown in the following four Figures (42-45) for LYSO 90/10. It may be observed that as the impact of Lu is higher and the absorption of incident x-ray photons is slightly increased, the number of produced and absorbed K x-ray photons of Lu is increased, while that of Y is decreased.

Figure 42. Number of incident, absorbed x-ray and produced K-fluorescence x-ray photons versus x-ray energy for 34 mg/cm² of LYSO 90/10, calculated by Monte Carlo.
Figure 43. Number of absorbed x-ray and absorbed K-fluorescence x-ray photons versus x-ray energy for 34 mg/cm² of LYSO 90/10, calculated by Monte Carlo.

Figure 44. Number of incident, absorbed x-ray and produced K-fluorescence x-ray photons versus coating thickness of LYSO 90/10 and for constant x-ray energy (65 keV), calculated by Monte Carlo.
Figure 45. Number of absorbed x-ray and absorbed K-fluorescence x-ray photons versus coating thickness of LYSO 90/10 and for constant x-ray energy (65 keV), calculated by Monte Carlo.

Figure 46 shows the variation number of incident and absorbed x-ray photons with x-ray energy for a particular coating thickness (34 mg/cm$^2$) of CsI scintillator. Also, it depicts the variations of the number of produced K x-ray photons of Cs and I elements in the energy range from 20 up to 160 keV. As it was mentioned before, the produced K x-ray photons of Cs cannot produce additional K x-ray photons of I.

Figure 46. Number of incident, absorbed x-ray and produced K-fluorescence x-ray photons versus x-ray energy for 34 mg/cm$^2$ of CsI, calculated by Monte Carlo.

Figure 47 depicts the corresponding absorbed K x-ray photons for the parameters investigated in Figure 46.
Figure 47. Number of absorbed x-ray and absorbed K-fluorescence x-ray photons versus x-ray energy for 34 mg/cm$^2$ of CsI, calculated by Monte Carlo.

Figure 48 illustrates variations of the parameters shown in Figure 46. The difference in this case, is that the variations are proportional to the coating thickness of CsI scintillator, for a constant incident x-ray photon energy (40 keV).

Figure 48. Number of incident, absorbed x-ray and produced K-fluorescence x-ray photons versus coating thickness of CsI and for constant x-ray energy (40 keV), calculated by Monte Carlo.

Figure 49 shows the same parameters depicted in Figure 47, proportional to CsI scintillator’s coating thickness for a constant incident x-ray photon energy (40 keV).
Figure 49. Number of absorbed x-ray and absorbed K-fluorescence x-ray photons versus coating thickness of CsI and for constant x-ray energy (40 keV), calculated by Monte Carlo.

Figure 50 shows the variation number of incident and absorbed x-ray photons with x-ray energy for a particular coating thickness (34 mg/cm$^2$) of YTaO$_4$ scintillator. Also, it depicts the variations of the number of produced K x-ray photons of Ta (K$_{Ta}$), the K x-ray photons of Y because of incident x-ray photons (K$_{Y/\text{inc}}$) and the K-photons of Y because of the produced K x-ray photons of Ta (K$_{Y/Ta}$). Finally, it shows the total number of produced K x-ray photons of Y (K$_{Y}$) in the energy range from 20 up to 160 keV. For the same x-ray energy the number of produced K x-ray photons of Ta is higher than the number of produced K x-ray photons of Y. This happens due to the reasons mentioned in LYSO 50/50 scintillator’s case. Also, for the same parameters the number of K$_{Y/\text{inc}}$ is higher than the respective number of K$_{Y/Ta}$. However, the number of K$_{Y/Ta}$ increases rapidly with coating thickness, due to the increase of the production of K x-rays of Ta and their reabsorption from Y element.
Figure 50. Number of incident, absorbed x-ray and produced K-fluorescence x-ray photons versus x-ray energy for 34 mg/cm² of YTaO₄, calculated by Monte Carlo.

Figure 51 illustrates the corresponding absorbed K x-ray photons for the parameters investigated in the above figure. It may be observed that the number of absorbed K x-ray photons of Y element is slightly lower than the respective of Ta, despite the big difference between the two elements in the production of K x-ray photons. This happens because the produced K x-ray photons of Ta have higher average energy (57.22 keV) than that of Y element (14.89 keV), consequently they have higher tendency to escape the scintillator.
Figure 52 depicts variations of the parameters presented in Figure 50. The difference in this case, is that the variations are proportional to the coating thickness of YTaO$_4$ scintillator, for a constant incident x-ray photon energy (70 keV).

![Figure 52](image)

**Figure 52.** Number of incident, absorbed x-ray and produced K-fluorescence x-ray photons versus coating thickness of YTaO$_4$ and for constant x-ray energy (70 keV), calculated by Monte Carlo.

Figure 53 depicts the same parameters depicted in Figure 51, proportional to YTaO$_4$ scintillator’s coating thickness for a constant incident x-ray photon energy (70 keV).

![Figure 53](image)

**Figure 53.** Number of absorbed x-ray and absorbed K-fluorescence x-ray photons versus coating thickness of YTaO$_4$ and for constant x-ray energy (70 keV), calculated by Monte Carlo.
E.3 K-Factor

Figure 54 shows the variation of K-Factor with regard to x-ray energy, for constant coating thickness (60 mg/cm$^2$) of LSO scintillator. It may be observed that the K-Factor is defined for energies higher than the K-absorption edge energy of Lu. In this energy range, it has almost constant values. This happens because the average energy of K x-ray photons of Lu has specific value (53.79 keV) regardless of the incident x-ray photon energy. Therefore, the K x-ray photons of Lu have a prescribed probability to escape the scintillator.

![Figure 54. K-Factor (%) versus x-ray energy for 60 mg/cm$^2$ of LSO, calculated by Monte Carlo.](image)

Figure 55 depicts the variation of the K-Factor regarding the coating thickness, for LSO and for constant x-ray energy (65 keV). K-Factor decreases with the increase of coating thickness. This occurs because the K-Factor is a parameter inversely proportional to K x-ray reabsorption, which increases with the increase of coating thickness.

![Figure 55. K-Factor (%) versus coating thickness for LSO and for constant x-ray energy (65 keV), calculated by Monte Carlo.](image)
Figure 56 illustrates the variation of K-Factor with x-ray energy, for constant coating thickness (60 mg/cm²) of YSO scintillator. In this case, K-Factor is defined for energies higher than the K-absorption edge energy of Y.

![Figure 56. K-Factor (%) versus x-ray energy for 60 mg/cm² of YSO, calculated by Monte Carlo.](image)

Figure 57 shows the variation of K-Factor with reference to coating thickness, for YSO and for constant x-ray energy (20 keV).

![Figure 57. K-Factor (%) versus coating thickness for YSO and for constant x-ray energy (20 keV), calculated by Monte Carlo.](image)

Figure 58 shows the variation of K-Factors with regard to x-ray energy, for constant coating thickness (60 mg/cm³) of LYSO 50/50. K-Factor of Lu is higher than that of both Y/inc and Y/Lu. This happens because the average energy of K characteristic of Lu (53.79 keV) is higher than that of Y (14.89 keV). Thus, K x-ray photons of Y have higher probability to be
reabsorbed within the scintillator. Finally, the K-Factor of Y/inc is almost the same with that of Y/Lu. This occurs because the average energy of K-fluorescence radiation of Y is constant (14.89 keV), regardless of the way of K x-ray photons production.

Figure 58. K-Factor (%) versus x-ray energy for 60 mg/cm² of LYSO 50/50, calculated by Monte Carlo.

Figure 59 depicts the variation of K-Factor with coating thickness, for LYSO 50/50 and for constant incident x-ray energy (65 keV).

Figure 59. K-Factor (%) versus coating thickness for LYSO 50/50 and for constant x-ray energy (65 keV), calculated by Monte Carlo.
Figures 60 and 61 illustrate relevant variations with Figures 58 and 59, for LYSO 90/10.

![Graph of K-Factor (%) versus x-ray energy for 60 mg/cm² of LYSO 90/10, calculated by Monte Carlo.](image)

**Figure 60.** K-Factor (%) versus x-ray energy for 60 mg/cm² of LYSO 90/10, calculated by Monte Carlo.

![Graph of K-Factor (%) versus coating thickness for LYSO 90/10 and for constant x-ray energy (65 keV), calculated by Monte Carlo.](image)

**Figure 61.** K-Factor (%) versus coating thickness for LYSO 90/10 and for constant x-ray energy (65 keV), calculated by Monte Carlo.

Figure 62 presents a comparison of K-Factor values corresponding to LYSO 50/50 and LYSO 90/10 under the same conditions (coating thickness equal to 60 mg/cm² in the energy range from 5 up to 160 keV). In the case of LYSO 90/10, the K-Factors of Y/inc and Y/Lu decrease in comparison with the respective of LYSO 50/50. This takes place because the fraction of Lu increases, so there is an increased probability for K x-rays photons of Y to interact with the Lu element’s L-shell. On the other hand, the K-Factor values of Lu are almost the same in the two LYSO scintillators. This happens because there is a very small difference in their probability to be absorbed either by the K-absorption edge of Y, or by the L-absorption
edge of Lu element (they have identical attenuation coefficients for energies up to the K-absorption edge energy of Lu).

Figure 62. Comparison of LYSO 50/50 and the LYSO 90/10 for the K-Factor (%) of the same coating thickness (60 mg/cm²), calculated by Monte Carlo.

Figure 63 shows the variation of K-Factors with regard to x-ray energy, for constant coating thickness (60 mg/cm²) of CsI scintillator. For the reasons mentioned before, it may be observed that K-Factor of I due to the produced K x-ray photons of Cs can not be defined (K-factor I/Cs). K-Factor of Cs is slightly higher than that of I/inc. This happens because the average energy of K characteristic of Cs (30.89 keV) is slightly higher than that of I (28.51 keV). Thus, the K x-ray photons of I have a slightly higher probability to be reabsorbed within the scintillator.

Figure 63. K-Factor (%) versus x-ray energy for 60 mg/cm² of CsI, calculated by Monte Carlo.
Figure 64 depicts the variation of K-Factor with coating thickness, for CsI scintillator and for constant incident x-ray energy (40 keV).

![Graph](image1)

**Figure 64.** K-Factor (%) versus coating thickness for CsI and for constant x-ray energy (40 keV), calculated by Monte Carlo.

Figure 65 illustrates the variation of K-Factors regarding the x-ray energy, for constant coating thickness (60 mg/cm²) of YTaO₄ scintillator. K-Factor of Ta is higher than that of both Y/inc and Y/Ta for reasons explained in LYSO 50/50 scintillator’s case.

![Graph](image2)

**Figure 65.** K-Factor (%) versus x-ray energy for 60 mg/cm² of YTaO₄, calculated by Monte Carlo.

Finally, Figure 66 shows the variation of K-Factor with regard to coating thickness, for YTaO₄ scintillator and for constant incident x-ray energy (70 keV).

![Graph](image3)

**Figure 66.** K-Factor (%) versus coating thickness for YTaO₄ and for constant incident x-ray energy (70 keV).
Figure 66. K-Factor (%) versus coating thickness for YTaO₄ and for constant x-ray energy (70 keV), calculated by Monte Carlo.

E.4 Probabilities for K x-ray photons (PKA, PKI and PKR)

Figure 67 shows the variations of PKA, PKI and PKR of Lu element versus x-ray energy for a constant coating thickness (60 mg/cm²) of LSO scintillator. The PKA calculated by Monte Carlo was found to have constant values, regardless of the x-ray energy. On the other hand, the respective theoretical curve decreases with the increase of energy. This happens since the Monte Carlo model determines the PKA using the fraction of produced K x-ray photons over the x-ray photons absorbed by the scintillator (interacted through Photoelectric absorption which leads to totally energy deposition). On the contrary, the theoretical formula (12) calculates the PKA using the fraction of produced K x-ray photons over the interacting x-ray photons (through Photoelectric, Compton or Rayleigh interactions). Scattering interactions have very little contribution to attenuation probability for low energies. However, their contribution increases with the increase of energy. Therefore, the theoretically described PKA decreases as the x-ray energy increases. Hence, it may be assumed that the present Monte Carlo method gives more accurate values for this parameter. This is because it takes into consideration the probability per absorbed x-ray. The PKI calculated by Monte Carlo has almost identical values with those calculated by the theoretical formula (14). Hence, both Monte Carlo and theoretical models describe this parameter more or less accurately. Finally, it was observed that the Monte Carlo calculated PKR had lower values with respect to those calculated by the theoretical formula (17). This could be probably attributed to the limitations
of theoretical model. The absolute relative differences between Monte Carlo and theoretical calculations for PKA, PKI and PKR parameters were 11.61, 1.75 and 51.06 %, respectively.

![Figure 67](image1.png)

Figure 67. PKA, PKI and PKR versus x-ray energy. Comparison between Monte Carlo values (MC) and theoretical methods (TH) for 60 mg/cm² of LSO scintillator

Figure 68 depicts the variations of PKA, PKI and PKR of Y element regarding the x-ray energy for a constant coating thickness (60 mg/cm²) of YSO scintillator. Theoretical calculated PKA decreases rapidly with the increase of x-ray energy. This occurs because YSO scintillator has a relatively low-Z heavy element, so the scattering contribution to attenuation probability starts to increase in low energy (just after the K-absorption edge energy of Y-17.04 keV). The absolute relative differences between Monte Carlo and theoretical calculations for PKA, PKI and PKR parameters were found to be 43.03, 2.74 and 17.25 %, respectively.

![Figure 68](image2.png)

Figure 68. PKA, PKI and PKR versus x-ray energy. Comparison between Monte Carlo values (MC) and theoretical methods (TH) for 60 mg/cm² of YSO scintillator
Figure 69 illustrates the variations of PKA, PKI and PKR of Lu element with x-ray energy for a constant coating thickness (60 mg/cm^2) of LYSO 50/50 scintillator. The first two parameters were calculated by both Monte Carlo and theoretical models. PKR parameter didn’t calculated by the theoretical formula (17), because this formula is used for one heavy element scintillator. For phosphors with two heavy elements there is a more complicated formula, which is out of the present investigation’s interest. The absolute relative differences between Monte Carlo and theoretical calculations for PKA and PKI parameters were found to be 15.72 and 1.95 %, respectively.

![Figure 69. PKA, PKI and PKR of Lu versus x-ray energy. Comparison between Monte Carlo values (MC) and theoretical methods (TH) for 60 mg/cm^2 of LYSO 50/50 scintillator](image)

Figure 70 depicts the variations of PKA, PKI and PKR of Y element (for K x-rays of Y due to the incident x-ray photons) with x-ray energy for a constant coating thickness (60 mg/cm^2) of LYSO 50/50 scintillator. The first two parameters were calculated by both Monte Carlo and theoretical models. The sudden fall of PKA values happens due to the probability of Lutetium’s K x-ray photons generation. Therefore, there is a smaller probability for Yttrium’s K x-ray photons generation. The absolute relative differences between Monte Carlo and theoretical calculations for PKA and PKI parameters were 14.25 and 2.70 %, respectively.
Figure 70. PKA, PKI and PKR of Y/inc versus x-ray energy. Comparison between Monte Carlo values (MC) and theoretical methods (TH) for 60 mg/cm² of LYSO 50/50 scintillator.

Figure 71 shows the variations of PKA, PKI and PKR of Y element in relation to the produced K x-ray photons of Lu (for K x-rays of Y due to the produced K x-ray photons of Lu) versus x-ray energy for a constant coating thickness (60 mg/cm²) of LYSO 50/50 scintillator. All parameters were calculated only by Monte Carlo methods, because the respective theoretical formulas are complicated and out of the present investigation’s interest.

Figure 71. PKA, PKI and PKR of Y/Lu versus x-ray energy for 60 mg/cm² of LYSO 50/50 scintillator, calculated by Monte Carlo methods.

Figure 72 presents the variations of PKA, PKI and PKR of Lu element with regard to x-ray energy for a constant coating thickness (60 mg/cm²) of LYSO 90/10 scintillator. The first two parameters were calculated by both Monte Carlo and theoretical models. The absolute relative
differences between Monte Carlo and theoretical calculations for PKA and PKI parameters were found to be 12.1 and 1.82 %, respectively.

Figure 72. PKA, PKI and PKR of Lu versus x-ray energy. Comparison between Monte Carlo values (MC) and theoretical methods (TH) for 60 mg/cm² of LYSO 90/10 scintillator

Figure 73 depicts the variations of PKA, PKI and PKR of Y element (for K x-rays of Y due to the incident x-ray photons) versus x-ray energy for a constant coating thickness (60 mg/cm²) of LYSO 90/10 scintillator. The first two parameters were calculated by both Monte Carlo and theoretical models. The absolute relative differences between Monte Carlo and theoretical calculations for these parameters were 13.23 and 4.31 %.

Figure 73. PKA, PKI and PKR of Y/inc versus x-ray energy. Comparison between Monte Carlo values (MC) and theoretical methods (TH) for 60 mg/cm² of LYSO 90/10 scintillator
Figure 74 shows the variations of PKA, PKI and PKR of Y element in relation to the produced K x-ray photons of Lu (for K x-rays of Y due to the produced K x-ray photons of Lu) versus x-ray energy for a constant coating thickness (60 mg/cm²) of LYSO 90/10 scintillator.

It may be observed that the probabilities for K x-ray photons (PKA, PKI and PKR) of Lu element are higher in LYSO 90/10 scintillator. On the other hand, the respective probabilities for K x-ray photons of both Y/inc and Y/Lu are higher in LYSO 50/50 phosphor. This happens because in LYSO 90/10 scintillator the contribution of Lu element is higher, so there are smaller probabilities for generation and reabsorption of Yttrium’s K x-ray photons.

Figure 75 illustrates the variations of PKA, PKI and PKR of Cs element with x-ray energy for a constant coating thickness (60 mg/cm²) of CsI scintillator. The absolute relative differences between Monte Carlo and theoretical calculations for PKA and PKI parameters were found to be 17.14 and 2.06 %, respectively.
Figure 75. PKA, PKI and PKR of Cs versus x-ray energy. Comparison between Monte Carlo values (MC) and theoretical methods (TH) for 60 mg/cm² of CsI scintillator.

Figure 76 shows the variations of PKA, PKI and PKR of I element with x-ray energy for a constant coating thickness (60 mg/cm²) of CsI scintillator. The absolute relative differences between Monte Carlo and theoretical calculations for PKA and PKI parameters were 16.75 and 1.72 %, respectively.

Figure 76. PKA, PKI and PKR of I versus x-ray energy. Comparison between Monte Carlo values (MC) and theoretical methods (TH) for 60 mg/cm² of CsI scintillator.

Figure 77 presents the variations of PKA, PKI and PKR of Y element (for K x-rays of Y due to the incident x-ray photons) versus x-ray energy for a constant coating thickness (60 mg/cm²) of YTaO₄ scintillator. The first two parameters were calculated by both Monte Carlo...
and theoretical models. The absolute relative differences between Monte Carlo and theoretical calculations for these two parameters were found to be 11.91 and 2.05 %, respectively.

![Figure 77. PKA, PKI and PKR of Y/inc versus x-ray energy. Comparison between Monte Carlo values (MC) and theoretical methods (TH) for 60 mg/cm² of YTaO₄ scintillator](image)

Figure 77 depicts the variations of PKA, PKI and PKR of Ta element with regard to x-ray energy for a constant coating thickness (60 mg/cm²) of YTaO₄ scintillator. The absolute relative differences between Monte Carlo and theoretical calculations for PKA and PKI parameters were found to be 13.36 and 1.53 %, respectively.

![Figure 78. PKA, PKI and PKR of Ta versus x-ray energy. Comparison between Monte Carlo values (MC) and theoretical methods (TH) for 60 mg/cm² of YTaO₄ scintillator](image)
Figure 79 shows the variations of PKA, PKI and PKR of Y element in relation to the produced K x-ray photons of Ta (for K x-rays of Y due to the produced K x-ray photons of Ta) versus x-ray energy for a constant coating thickness (60 mg/cm²) of YTaO₄ scintillator.

![Figure 79. PKA, PKI and PKR of Y/Ta versus x-ray energy. Comparison between Monte Carlo values (MC) and theoretical methods (TH) for 60 mg/cm² of YTaO₄ scintillator](image)

E.5 Spatial distribution of the absorbed K x-ray photons (number and energy)

Figure 80 shows the spatial distribution of the absorbed K x-ray photon energy for 60 mg/cm² of LSO scintillator at energy of incident x-ray photons close to K absorption edge energy of Lu element (65 keV close to 63.31 keV). This happens because the purpose of this parameter’s study is to investigate the K x-ray photons influence at its higher value.

![Figure 80. Spatial distribution of the absorbed K x-ray photon energy for 60 mg/cm² of LSO scintillator at 65 keV.](image)
Figure 81 presents the spatial distribution of the absorbed K x-ray photon energy for 60 mg/cm² of YSO scintillator at energy of incident x-ray photons close to K absorption edge energy of Y element (20 keV close to 17.04 keV).

![Graph of Figure 81](image1)

**Figure 81.** Spatial distribution of the absorbed K x-ray photon energy for 60 mg/cm² of YSO scintillator at 20 keV.

Figure 82 depicts the spatial distribution of the absorbed K x-ray photon energy for 60 mg/cm² of LYSO 50/50 scintillator at energy of incident x-ray photons close to K absorption edge energy of Lu element (65 keV close to 63.31 keV).

![Graph of Figure 82](image2)

**Figure 82.** Spatial distribution of the absorbed K x-ray photons energy for 60 mg/cm² of LYSO 50/50 scintillator at 65 keV.

Figure 83 illustrates the spatial distribution of the absorbed K x-ray photon energy for 60 mg/cm² of LYSO 90/10 at 65 keV, respectively.

![Graph of Figure 83](image3)
Figure 83. Spatial distribution of the absorbed K x-ray photons energy for 60 mg/cm\(^2\) of LYSO 90/10 scintillator at 65 keV.

Figure 84 presents the spatial distribution of the absorbed K x-ray photon energy for 60 mg/cm\(^2\) of CsI scintillator at energy of incident x-ray photons close to K absorption edge energy of Cs element (40 keV close to 35.98 keV).

Figure 84. Spatial distribution of the absorbed K x-ray photon energy for 60 mg/cm\(^2\) of CsI scintillator at 40 keV.

Figure 85 depicts the spatial distribution of the absorbed K x-ray photon energy for 60 mg/cm\(^2\) of YTaO\(_4\) scintillator at energy of incident x-ray photons close to K absorption edge energy of Ta element (70 keV close to 67.42 keV).
Figure 85. Spatial distribution of the absorbed K x-ray photon energy for 60 mg/cm² of YTaO₄ scintillator at 70 keV.

Figure 86 shows the spatial distribution of the absorbed K x-ray photon energy for 60 mg/cm² of all scintillators at the aforementioned energies for each scintillator. It may be observed that LSO, LYSO 50/50, LYSO 90/10 and YTaO₄ scintillators have almost the same spatial distribution. This happens because of the presence of Lu and Ta elements, respectively. These two elements have almost the same average energy of K x-ray photons (53.79 keV and 57.22 keV respectively). Consequently, K x-ray photons of these two elements travel within the scintillator mass and are absorbed at relative distances. The small differences between the first three aforementioned scintillators are due to the fraction of Lu or Y elements inside the scintillator. LYSO 90/10 has slightly higher values than LSO, due to the presence of additional K x-ray photons of Y. On the other hand, LYSO 50/50 has lower values than LSO, because of the significantly lower production of K x-ray photons of Lu (the fraction of Y inside the scintillator is high). Both CsI and YSO scintillators have higher values at low distances and lower values at higher distances in comparison with the previous scintillators. This happens because they have elements which exhibit K x-ray photons of lower energy (30.89 and 28.51 keV for CsI and 14.89 keV for YSO). Therefore, they are absorbed more locally.
Finally, Figure 86 shows the respective spatial distribution of the absorbed K x-ray photons number for 60 mg/cm² of all scintillators at the aforementioned energies for each scintillator. The number of absorbed K x-ray photons of CsI is slightly lower than that of LSO, LYSO 50/50, LYSO 90/10 and YTaO₄ scintillators at higher distances. However, both YSO and CsI scintillators have higher values at lower distances (local absorption).
CHAPTER F

CONCLUSIONS AND FUTURE WORK

F.1 Conclusions ..................................................................................................................94
F.2 Future work .................................................................................................................95
F.1 Conclusions

In the present study a previously developed and validated Monte Carlo model, investigating the imaging properties of x-ray scintillators, was extended to include the effect of K-fluorescence emission on scintillators incorporating two heavy elements. Within the framework of this model some fundamental radiation detection properties of scintillators were first confirmed: a) the radiation detection ability increases with the atomic number Z of the heavy elements of the scintillator (such as LSO, LYSO and YTaO₄ scintillators), b) the probability of K x-ray photon generation also increases with atomic number. Furthermore, 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 YSO and CsI scintillators), absorb a larger fraction of the produced K x-ray photons than phosphors with high-Z heavy elements. 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.

The effect of additional K x-ray photons (e.g. those created in the low-Z element by the K x-rays of the high-Z element) is negligible on thin phosphor screens. On the contrary, it is considerably stronger in thicker scintillators. It is similar to the effect of K x-ray photons of low-Z heavy element. This is because the reabsorption of K x-ray photons emerging from the high Z element is higher in thick scintillators. This results to further production of additional K x-rays from the low-Z heavy element.

K x-ray photon lateral diffusion results in image blurring. In scintillators consisting of elements with relatively low-Z (YSO and CsI case), K x-ray photons are absorbed within small distances from the point of creation. In addition, the fraction of K-photons absorbed in these materials is higher. This may result in image blurring effects which extend to a limited range, however are more significant than those corresponding to high-Z scintillators (LSO, LYSO and YTaO₄). However, they are restricted into a limited range. Thus they may have no significant effect on the overall image blurring, mainly originating from light photons spread.

In the case of nuclear medicine imaging detectors, when high-Z scintillators are used, the system’s counting efficiency may have a more significant decrease. This is because a larger number of pulse amplitudes could fall outside the system’s energy window.
The YSO scintillator may be suitable for use in x-ray mammography since: a) it shows high detection ability at low energies and b) K x-ray photons are locally absorbed. On the other hand, LSO, LYSO, CsI and YTaO$_4$ scintillators may be considered suitable for higher energy imaging applications (general x-ray radiography, CT and nuclear medicine $\gamma$-ray imaging conditions). According to the investigated parameters, LYSO 90/10 presents better performance than LYSO 50/50. More specifically, for energies higher the K-edge of Lu (63.31 keV), LYSO 90/10 of 60 mg/cm$^2$ has approximately 16% higher detection efficiency in comparison with LYSO 50/50. On the other hand, LYSO 90/10 exhibits only 4% higher amount of K x-rays.

**F.2 Future work**

General purpose for the future work is to extend the model in order to make a more detailed investigation of the K-fluorescence effect on scintillators. This investigation may be achieved by the consideration of: (a) x-ray spectra used in medical imaging systems, (b) the effect of secondary electron range and (c) the simulation of light photon transport within the materials. A Computer cluster instead of a single-processor may help to achieve the aforementioned considerations.
## APPENDIX I: ABBREVIATIONS

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Full Form</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>Aluminum</td>
</tr>
<tr>
<td>CDF</td>
<td>Cumulative Distribution Function</td>
</tr>
<tr>
<td>Cs</td>
<td>Cesium</td>
</tr>
<tr>
<td>CsI</td>
<td>Cesium Iodide</td>
</tr>
<tr>
<td>fpl</td>
<td>free path length</td>
</tr>
<tr>
<td>Γ</td>
<td>gamma</td>
</tr>
<tr>
<td>I</td>
<td>Iodide</td>
</tr>
<tr>
<td>LSO</td>
<td>Lutetium Oxyorthosilicate</td>
</tr>
<tr>
<td>Lu</td>
<td>Lutetium</td>
</tr>
<tr>
<td>LYSO</td>
<td>Lutetium Yttrium Oxyorthosilicate</td>
</tr>
<tr>
<td>MC</td>
<td>Monte Carlo</td>
</tr>
<tr>
<td>Mo</td>
<td>Molybdenum</td>
</tr>
<tr>
<td>NIST</td>
<td>National Institute of Standards and Technology</td>
</tr>
<tr>
<td>PDF</td>
<td>Probability Density Function</td>
</tr>
<tr>
<td>PKA</td>
<td>Probability of K-fluorescence x-ray photon generation per Absorbed x-ray</td>
</tr>
<tr>
<td>PKI</td>
<td>Probability of K-fluorescence x-ray photon generation per Incident x-ray</td>
</tr>
<tr>
<td>PKR</td>
<td>Probability of generation and Reabsorption of a K x-ray per incident x-ray</td>
</tr>
<tr>
<td>Ta</td>
<td>Tantalum</td>
</tr>
<tr>
<td>TH</td>
<td>Theoretical</td>
</tr>
<tr>
<td>W</td>
<td>Tungsten</td>
</tr>
<tr>
<td>Y</td>
<td>Yttrium</td>
</tr>
<tr>
<td>YSO</td>
<td>Yttrium Oxyorthosilicate</td>
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</tbody>
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