MONTE CARLO SIMULATION OF THE RESPONSE FUNCTIONS OF CdTe DETECTORS TO BE APPLIED IN X-RAY SPECTROSCOPY

Alessandra Tomal, Alejandro H. Lopez Gonzales, Josilene C. Santos, Paulo R. Costa

1 Instituto de Física, Universidade Federal de Goiás, Campus Samambaia
74001-970, Goiânia, GO, Brazil
alessandra_tomal@yahoo.com.br

2 Instituto de Física da Universidade de São Paulo
Rua do Matão Travessa R.187CEP 05508-090 Cidade Universitária, São Paulo – Brazil
ahlopezg@uni.pe; josilene@usp.br; pcosta@if.usp.br

Abstract

In this work, the energy response functions of a CdTe detector were obtained by Monte Carlo (MC) simulation in the energy range from 5 to 150 keV, using the PENELOPE code. The response functions simulated included the finite detector resolution and the carrier transport. The simulated energy response matrix was validated through comparison with experimental results obtained for radioactive sources. In order to investigate the influence of the correction by the detector response at diagnostic energy range, x-ray spectra were measured using a CdTe detector (model XR-100T, Amptek), and then corrected by the energy response of the detector using the stripping procedure. Results showed that the CdTe exhibit good energy response at low energies (below 40 keV), showing only small distortions on the measured spectra. For energies below about 70 keV, the contribution of the escape of Cd- and Te-K x-rays produce significant distortions on the measured x-ray spectra. For higher energies, the most important correction is the detector efficiency and the carrier trapping effects. The results showed that, after correction by the energy response, the measured spectra are in good agreement with those provided by different models from the literature. Finally, our results showed that the detailed knowledge of the response function and a proper correction procedure are fundamental for achieve more accurate spectra from which several qualities parameters (i.e. half-value layer, effective energy and mean energy) can be determined.

Keywords: X-ray spectra, Response functions, CdTe detector
1.- INTRODUCTION

The knowledge of the energy distribution of photons produced by an x-ray tube is an important task for optimization and development of imaging system, dosimetry and radiation protection (Wilkinson et al., 2001; Kunzel et al., 2004; Cunha et al., 2012). The standard method for determine experimentally the photon energy distribution of radiation field produced by x-ray tubes is the x-ray spectroscopy performed using high resolution semiconductor detectors, followed by a proper correction procedure by the energy response of the detector (Di Castro et al., 1984; O’Foghludha and Johnson, 1981, Matsumoto et al., 2000; Wilkinson et al., 2001; Miyajima and Imagawa, 2002; Kunzel et al., 2004; Abbene et al., 2007; Tomal et al., 2011, 2012).

Recently, measurements of x-ray spectra at diagnostic energy range have been performed with portable CZT and CdTe detectors (Miyajima and Imagawa, 2002; Kunzel et al., 2004; Bottigli et al., 2006; Abbene et al., 2007). These detectors have several advantages for x-ray spectroscopy due to its high atomic number and high detection efficiency. Besides, they have small dimensions due to the refrigeration by Peltier effect, which allows spectra measurements under clinical conditions. However, the spectra measured with CZT and CdTe detectors show greater spectral distortions compared with that obtained with HPGe and Si(Li), which is related with the higher probability of escape of fluorescent x-rays and with their poor carrier transport. Besides, the spectra measured with the CdTe detector show smaller spectral distortions compared to that measured with the CZT due to its small carrier trapping probability (Miyajima and Imagawa, 2002), although these distortions can not be neglect. Thus, a proper and detailed determination of the response of the CdTe detector is need, in order to correct properly the measured x-ray spectra with this detector.

In this work, the energy response functions of a CdTe detector were obtained by Monte Carlo (MC) simulation in the energy range from 5 to 160 keV, using the PENELLOPE code. The response functions simulated were based in previous works and included the finite
detector resolution and the carrier transport. The simulated energy response matrix was validated through comparisons with experimental results obtained for radioactive sources ($^{241}$Am and $^{152}$Eu). In order to investigate the influence of the correction by the detector response at different tube potential range, x-ray spectra were measured using a CdTe detector and corrected by its energy response using the stripping procedure.

2.- MATERIAL AND METHODS

2.1.- Determination of detector response

The response functions were calculated through Monte Carlo (MC) simulations, using the PENELOP code version 2003 (Salvat et al, 2003). The incident radiation was assumed to be a monoenergetic pencil beam from 5 to 160 keV, at 0.5 keV intervals. For each incident energy, $10^6$ photons were simulated. The geometrical mathematical model used for the simulation of the CdTe detector was based on the information provided by the manufacturers, which consisted of a CdTe crystal, with thickness of 1 mm and 9 mm$^2$ area, located behind a Be window of 100 µm and sandwiched between two electrodes made of platinum (0.2 µm, cathode) and indium (0.1 µm, anode).

The simulation of the detector response was based in a previous work (Tomal et al, 2012), which consisted in follow the history of each incident photon, as well as secondary photons and electrons, until their energy is higher than a cutoff value (0.5 keV). For each interaction inside the detector’s crystal, the deposited energy was determined by considering the position of interaction and including the carrier transport and the finite energy resolution (Tomal et al, 2011, 2012). These effects were modeled through the inclusion of specific features of the detector: (a) carrier trapping effects, modeled by the Hecht equation (Cross et al, 2005; Moralles et al, 2007); (b) the incomplete charge collection (ICC), modeled by the Carrier collection probability (CCP) function (Campbell et al, 2001); and (c) the
detector energy resolution, modeled by a Gaussian sampling of the deposited energy (Campbell et al, 1998). The input data of the Hecht equation and of the CCP function used to simulate the effects (a) and (b), respectively, are summarized in Table 1. These parameters were determined to achieve the best coincidence between the simulated and experimental spectra of radioactive sources (Matsumoto et al, 2000; Tomal et al, 2012). Table 1 also includes the dead layer thickness used in the simulation, which were adjusted to provide the best agreement between the simulated and experimental data for radioactive sources (Moralles et al, 2007). The input data of the Gaussian distribution, relating the Gaussian peak width with the photon energy (Campbell et al, 1998, 2001), were adjusted from the experimental resolution curve, obtained using radioactive sources (Mesradi et al, 2008).

Table 1.- Parameter of the Hecht equation and CCP function, and dead layer user in MC simulation of CdTe detector

<table>
<thead>
<tr>
<th>$\lambda_c$ (cm)</th>
<th>$\lambda_h$ (cm)</th>
<th>$D/\nu$ (µm)</th>
<th>$RC$</th>
<th>$d_L$ (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>12.5</td>
<td>0.78</td>
<td>0.2</td>
<td>0.2</td>
<td>3.0</td>
</tr>
</tbody>
</table>

2.2.- X-ray spectra measurements

The x-ray spectra were generated by an industrial x-ray tube with a stationary tungsten (W) target (model MG 450, Philips), with anode angle of 22°, and a 2.2 mm beryllium (Be) exit window. The x-ray tube is powered by a constant-potential generator, operating at constant tube potentials between 40 and 150 kVp, and adapted with additional filters of Al with 99.9% of purity to comply to the standard beam qualities recommended by the IEC 61267.

The spectra were measured with a CdTe diode detector (Amptek, model XR-100T CdTe), with thickness of 1 mm and 9 mm$^2$ nominal area, and a Be window of thickness 100 µm. The pulses from the detector were processed by an Amptek PX4 amplifier. The nominal bias voltage was 400 V. The energy calibration and the resolution of the each detection
system were determined by using the and the x- spectra of radioactive sources of $^{241}$Am and $^{152}$Eu. For these measurements, a 2 mm thick tungsten collimator with a 0.5 mm diameter aperture was utilized at a distance of 3 cm from the detector window.

The measurements of x-ray spectra were made at a distance of 3.7 m from the focus. A tungsten pinhole collimator (2 mm thick and 0.5 mm diameter) was utilized in front of each detector in order to reduce the fluence rate, and consequently, pile up effects and dead time losses on the x-ray spectra. The rise time discrimination (RTD) circuit of all detectors was switched off during the measurements (Miyajima, 2003). Measured x-ray spectra were corrected by the response of the CdTe detector, using the stripping method (Di Castro et al, 1984; Tomal et al, 2011).

### 3.- RESULTS

#### 3.1.- Response functions

Figure 1 compares the experimental and simulated $^{241}$Am spectra for the CdTe detector. Both spectra are normalized for the same peak intensity.
Figure 1.- Simulated and measured $^{241}$Am spectra obtained with the CdTe detector.

Figure 1 shows a good agreement between the experimental and simulated $^{241}$Am spectra obtained with the CdTe detector, indicating the suitability of Monte Carlo simulation for modeling the response of semiconductor detectors and the good choice of the input parameters used.

Figure 2 shows the monoenergetic response functions for the CdTe detector at 40 keV, 70 keV and 160 keV.

Figure 2 shows that the heights of the main peaks decrease with the energy increasing, indicating that the distortions due the transmission of primary x-rays are greater for high energies. The tail and flat-shelf contributions to the total response also increase with the energy increasing, due to the higher hole trapping. Besides, the escape of characteristic K x-rays from Cd and Te is also an important contribution to the response function of this detector, since it distorts the spectra towards the low energies region (Miyajima and Imagawa, 2002). However, this contribution decreases with the energy increasing.
Figure 3 shows the full-energy peak efficiency for the CdTe detector, computed from the simulated response functions. The values were computed by including or neglecting the carrier transport effects (carrier trapping and charge reflection).

![Graph showing full-energy peak efficiency for the CdTe detector.](image)

Figure 3 shows that both full-energy peak efficiencies curves for the CdTe detector, computed by including or neglect the carrier transport effects, have a similar dependence with the photon energy. The full-energy peak efficiency is maximum for energies between 10-27 keV, but it presents edges at 26.7 keV and 31.8 keV (Miyajima, 2003), which is related to the K-edges of linear attenuation coefficient of Cd and Te. Besides, for energies greater than 50 keV the full-energy peak efficiency decreasing rapidly. Moreover, the differences between the efficiencies determined by including or neglecting the carrier transport effects are small for energies lesser than approximately 40 keV. For energies greater than 40 keV, the efficiency is significantly reduced by including the carrier transport effects, mainly due to worst hole transport. Thus, spectral corrections due to efficiency of CdTe detector are very important for energies higher than 27 keV (Kunzel et al, 2004; Tomal et al, 2012).
The escape fraction of K-fluorescents radiation for the CdTe detector, computed from the simulated response functions, are shown in Figure 4 as a function of the incident energy.

![Graph showing escape fractions for CdTe detector](image)

Figure 4.- Simulated K-escape fractions for the CdTe detector.

Figure 4 shows that the escape fractions for the K-α peaks are greater than for K-β peaks due to its greater emission probability (Di Castro et al, 1984). The escape fraction for the K-fluorescent peaks of cadmium and tellurium decreases with the incident photon energy, which is explained mainly due the decreases of the probability of photoelectric effect with energy increasing. As shown in Figure 4, the spectral corrections due to escape of fluorescent radiation for the CdTe detector are more important for energies from 26.8 keV to 80 keV.

### 3.2.- X-ray spectra

Figure 5 compares the measured and corrected x-ray spectra obtained with the CdTe detector for 100 kVp. The spectra were normalized to unit area.
Figure 5.- Measured and corrected x-ray spectra obtained with CdTe detectors for 100 kVp.

As showed in Figure 5, the correction procedure removes the spectral distortions at different energy range due to different physical effect observed on the response functions. The correction procedure removes the counts at low energies (< 20 keV) present in the measured spectra, which can be attributed to the Cd and Te characteristic x-rays escape and carrier trapping effect. Besides, the correction by the detector efficiency removes the dips between 26 and 31 keV and corrects the spectral distortions above 60 keV. As shown in Figure 5, the correction of measured x-ray spectra by the response functions of the CdTe detector is fundamental to obtain more realistic spectra.

4. DISCUSSIONS AND CONCLUSIONS

The results obtained in this work show that the code PENELOPE can be a useful tool to determine the energy response functions of semiconductor detectors, with a good agreement with experimental data obtained using radioactive sources.

Besides, the results showed that, after correction by the energy response, the measured spectra are in good agreement with those provided by different models from the literature.
Finally, our results showed that the detailed knowledge of the response function and a proper correction procedure are fundamental for achieve more accurate spectra from which several qualities parameters (i.e. half-value layer, effective energy and mean energy) can be determined.

Acknowledgements
This work was supported by the Brazilian agencies Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) and Fundação de Amparo à Pesquisa do Estado de São Paulo (FAPESP).

REFERENCES


Bottigli U; Golosio B; Masala GL; Oliva P; Stumbo S; Delogu P; Fantacci ME; Abbene L; Fauci F; Raso G. (2006). Comparison of two portable solid state detectors with an improved collimation and alignment device for mammographic x-ray spectroscopy. Medical Physics 33: 3469-3477.

Campbell JL; Cauchon G; Lepy MC; McDonald L; Plagnard J; Stemmler P; Teesdale WJ; White G. (1998). A quantitative explanation of low-energy tailing features of Si(Li) and Ge x-ray detectors, using synchrotron radiation. Nuclear Instruments and Methods A 418: 394–404.


Chen C; Doi K; Vyborny C; Chan HP; Holje G. (1980). Monte Carlo simulation studies of detectors used in the measurement of diagnostic x-ray spectra. Medical Physics 7: 627–635.


Kunzel R; Herdade SB; Terini RA; Costa PR. (2004). *X-ray spectroscopy in mammography with a silicon PIN photodiode with application to the measurement of tube voltage*. Medical Physics 31: 2996–3003.


Tomal A; Cunha DM; Antoniassi M; Poletti ME. (2012). *Response functions of Si(Li), SDD and CdTe detectors for mammographic x-ray spectroscopy*. Applied Radiation and Isotopes **70**: 1355–1359.