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Monte Carlo simulation of the response functions of CdTe detectors to be applied in x-ray spectroscopy

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HIGHLIGHTS

- The response function of a CdTe detector was determined by Monte Carlo simulation.
- The simulation takes into account all interaction process, the carrier transport and the Gaussian resolution.
- The influence of different effects of spectral distortion was investigated.
- CdTe detector was applied for x-ray spectroscopy.
- The proper correction procedure is needed to achieve realistic x-ray spectra.

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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 160 keV, using the PENELOPE code. In the response calculations the carrier transport features and the detector resolution were included. The computed energy response function was validated through comparison with experimental results obtained with ^{241}Am and ^{152}Eu 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 exhibits good energy response at low energies (below 40 keV), showing only small distortions on the measured spectra. For energies below about 80 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 a theoretical model of the literature. Finally, our results showed that the detailed knowledge of the response function and a proper correction procedure are fundamental for achieving more accurate spectra from which quality parameters (i.e., half-value layer and homogeneity coefficient) can be determined.

1. Introduction

The knowledge of the energy distribution of photons produced by an x-ray tube is an important prerequisite for many applications in several basic and applied research fields and in practical use of ionizing radiation, such as nuclear science, medical physics and radiation protection (Wilkinson et al., 2001; Künzel et al., 2004; Cunha et al., 2012). In particular, in medical physics, the detailed knowledge of x-ray spectra is fundamental for mathematical modeling of image quality and dose in medical imaging (Cunha et al., 2012; Tomal et al., 2011), as well as for development of new image and detection systems (Carton et al., 2009).

In practical situations, the information about the energy of a polyenergetic x-ray beam is provided by simplified beam quality parameters (i.e., half-value layer, effective energy and homogeneity coefficient) (Carlsson and Carlsson, 1984; Kharrati and Zarrad, 2003), which characterize the beam in terms of its ability to penetrate a given material. Despite these quality parameters can

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be easily determined using an ionization chamber and specific filters, they are not useful to provide the complete description of energy of an x-ray beam. The x-ray spectrum (i.e., photon fluence in each energy interval) constitutes the more complete representation of the x-ray beam, since it provides the detailed information about the distribution of photons with the quantity and the quality of the beam (Künzel et al., 2004; Kharrati and Zarrad, 2003). From the description of the energy distribution of the beam provided by the x-ray spectra, several quality parameters of the beam (i.e., HVL, mean energy, effective energy and homogeneity coefficient) can also be determined numerically (Carlsson and Carlsson, 1984; Kharrati and Zarrad, 2003) to be compared with those extracted in most practical applications.

The standard method to determine experimentally the photon energy distribution of the radiation field produced by x-ray tubes is direct x-ray spectroscopy performed using high-resolution semiconductor detectors. Nevertheless, experimental determination of x-ray spectra is a complex task, due to the spectral distortion due to the inherent detector efficiency, escape of secondary radiation, incomplete charge collection and carrier trapping effects (Di Castro et al., 1984; O'Foghludha and Johnson, 1981; Matsumoto et al., 2000; Wilkinson et al., 2001; Miyajima and Imagawa, 2002; Künzel et al., 2004; Abbene et al., 2007; Tomal et al., 2011, 2012). Thus, a common approach to accurate spectra determination is based on proper correction of the measured pulse-height distribution for the energy response function of the detector effects (Di Castro et al., 1984; Tomal et al., 2011)

In the last years, most of the measurements of x-ray spectra at diagnostic energy range have been performed with portable CdTe detectors (Miyajima and Imagawa, 2002; Künzel 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 the Peltier effect, which allows spectra measurements under clinical conditions. However, the spectra measured with CdTe detectors show greater spectral distortions compared with that obtained with HPGe and Si(Li), which is related to their worse energy resolution, higher probability of escape of fluorescent x-rays and poor carrier transport. Thus, a proper and detailed determination of the response of the CdTe detector is need in an extended energy range, in order to correct properly the measured x-ray spectra with this kind of detector. In a previous work (Tomal et al., 2012) we had studied the response functions of the CdTe detector for energies used in mammography including the carrier transport and finite energy resolution. However, due to the low energy of incident photons, the modeling of the carrier trapping effects is simplified, since the interaction of photons occur shallow in the detector crystal and the range of the secondary electrons is smaller than the detector thickness.

In this work, the energy response functions of a CdTe detector was obtained by Monte Carlo (MC) simulation in the energy range from 5 to 160 keV, using the PENELOPE code. The simulation of the response functions of the CdTe detector for the diagnostic energy range was based on previous works (Tomal et al., 2011, 2012) and included the finite detector resolution and the carrier transport. The simulated energy response functions were validated through comparisons with experimental results obtained with radioactive sources (^{241}Am and ^{152}Eu). In order to investigate the influence of the correction by the detector response at different tube potentials, x-ray spectra were measured using a CdTe detector and corrected by its energy response using the stripping procedure (Di Castro et al., 1984). Finally, from the uncorrected and corrected spectra, the half-value layer and homogeneity coefficients were computed, in order to compare with those obtained experimentally.

2. Material and methods

2.1. Determination of detector response

The response functions were calculated through Monte Carlo (MC) simulations, using the PENELOPE 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. The model geometric simulated also included the electrodes made of platinum (0.2 μm, cathode) and indium (0.1 μm, anode), located respectively in front and beside the CdTe crystal regarding the incident beam.

The simulation of the detector response was based on a previous work (Tomal et al., 2012), which consisted in following the history of each incident photon, as well as secondary photons and electrons, until their energy is lower than a cutoff value (0.5 keV). For each interaction inside the detector's crystal, the deposited energy was determined and it was related to the response of the detector by considering the position of the interaction. The response function for each incident energy was modeled by considering the deposited energy in the interaction of photon with the crystal (related to the number of electron–hole pairs created), the carrier transport (carrier trapping effects and incomplete charge collection) and the finite energy resolution (Tomal et al., 2011, 2012; Campbell et al., 1998, 2001; Cross et al., 2005; Moralles et al., 2007). These effects were modeled as described in previous works (Tomal et al., 2011, 2012).

The dead layer thickness and the input data used for modeling the carrier trapping effects and the incomplete charge collection were determined to achieve the best coincidence between the simulated and experimental spectra of radioactive sources, as described by Tomal et al. (2012). Table 1 summarizes these parameters used in the simulation. The experimental resolution curve, obtained using radioactive sources of ^{241}Am and ^{152}Eu (Mesradi et al., 2008), was used to take into account the finite energy resolution based on a Gaussian distribution (Campbell et al., 1998, 2001). The fitting parameters of a second order polynomial to the experimental resolution data correspond to the input to simulate the energy resolution ($\mathrm{FWHM} = a_0 + a_1 \times E + a_2 \times E$), where E is the photon energy. Table 1 summarizes all parameters used in the simulation.

For comparison, the experimental full-energy peak efficiency for the CdTe detector was also obtained using the method descried by Mesradi et al. (2008), and considering the sources' activities (286 ± 9) kBq and (390 ± 13) kBq for the ^{241}Am and ^{152}Eu sources, respectively.

Table 1
Parameters of the Hecht equation, carrier collection probability function, dead layer thickness and resolution curve used in the simulation of CdTe detector.

Parameter	Value
λ_e (cm)	12.5
λ_h (cm)	0.78
D/ν (μm)	0.2
RC	0.2
d_L (μm)	30.0
a_0 (keV)	0.24
a_1	4.6×10^{-3}
a_2 (keV^{-1})	6.9×10^{-6}

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 achieve to the standard beam qualities recommended by the International Electrotechnical Commission (IEC 61267, 2005).

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 detection system were determined by using the γ and the x-spectra of radioactive sources of ^{241}Am and ^{152}Eu. For these measurements, a 2 mm thick tungsten pinhole collimator with a 0.5 mm diameter aperture was utilized at a distance of 3 cm from the detector window (Miyajima, 2003).

The measurements of x-ray spectra were made at a distance of 3.7 m from the focus and corrected analytically by the air attenuation to represent the beam qualities defined by IEC 61267 at a distance of 1 m from focal spot. The same collimation system was utilized in front of 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 the detection system was switched off during the measurements (Miyajima, 2003). Measured x-ray spectra were corrected for the response of the CdTe detector, using the stripping method (Di Castro et al., 1984; Tomal et al., 2011).

2.3. Determination of quality parameters from the corrected spectra

The HVL values and the homogeneity coefficients (HC) were computed from the uncorrected and corrected spectra obtained using the CdTe detector (Kharrati and Zarrad, 2003; Künzel et al., 2004). The computed values were compared to those determined experimentally using an ionization chamber (PTW, model 23361), coupled to an electrometer (PTW, model Unidos E).

3. Results and discussions

3.1. Response functions

Fig. 1 compares the experimental and simulated ^{241}Am spectra for the CdTe detector to validate the MC code modified to include the specific features of the detector. For comparison, both spectra are normalized for the same peak intensity. From Fig. 1, it can be observed as the γ and the x-peaks from the ^{241}Am source (1), as well as the Cd and Te K-escape peaks related to the 59.5 keV incident photons (2). The uncertainties were estimated based on the Poisson statistics being smaller than 3% and 1% in the measured and simulated spectra, respectively. In a general way, it was observed that a good agreement between the experimental and simulated ^{241}Am spectra obtained with the CdTe detector, with a coefficient of determination $R^2 = 0.99$. Besides, the experimental and simulated spectra of radioactive sources showed differences up to 10% in the main and escape peaks areas.

Fig. 2 shows the monoenergetic response functions for the CdTe detector at 35 keV, 90 keV and 150 keV, smothered to reduce the noise. From Fig. 2, it can be observed that the height of the main peaks decrease when the energy increases, indicating that the distortions due to the transmission of primary x-rays are

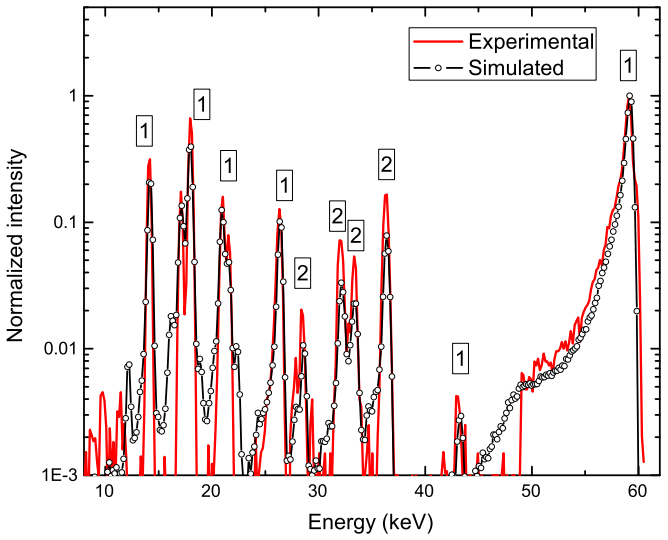

Fig. 1. Simulated and measured ^{241}Am spectra obtained with the CdTe detector. Labels (1) indicate the main peaks corresponding to the γ- and the x-ray lines emitted by the ^{241}Am source and labels (2) correspond to the Cd and Te K-escape peaks related to the 59.5 keV incident photons.

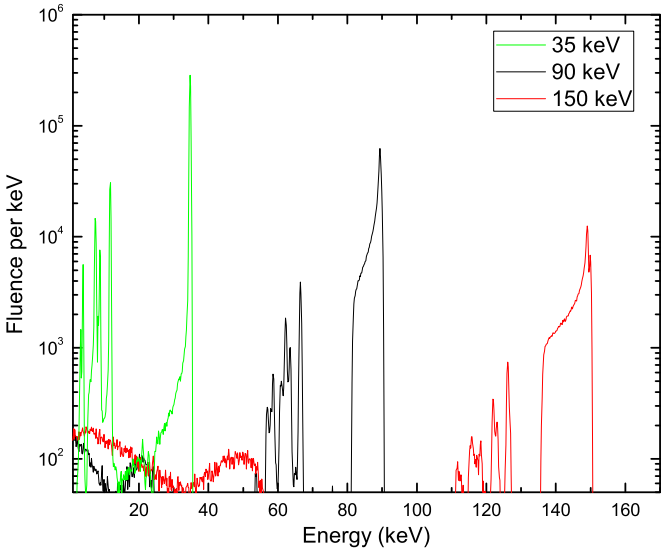

Fig. 2. Simulated monoenergetic response functions for the CdTe detector at 35 keV, 90 keV and 150 keV.

greater for high energies, which is explained by the lower attenuation of the radiation with higher energy. With the energy increase, the tail and flat-shelf contributions to the total response also increase with the incident energy increasing, due to the hole trapping effect. This effect reduces the height of the main peak and distorts the spectra toward the energies below the main peak, adding counts at energies up to approximately 20 keV below the incident energy. 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 region of energies below the main peak (Miyajima and Imagawa, 2002), i.e., around 26–32 keV below the incident energy. However, the contribution of the escape of characteristic decreases when the energy increases, being smaller than 5% for energies above 80 keV.

Fig. 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). Fig. 3 also includes the experimental values of full-peak energy efficiency

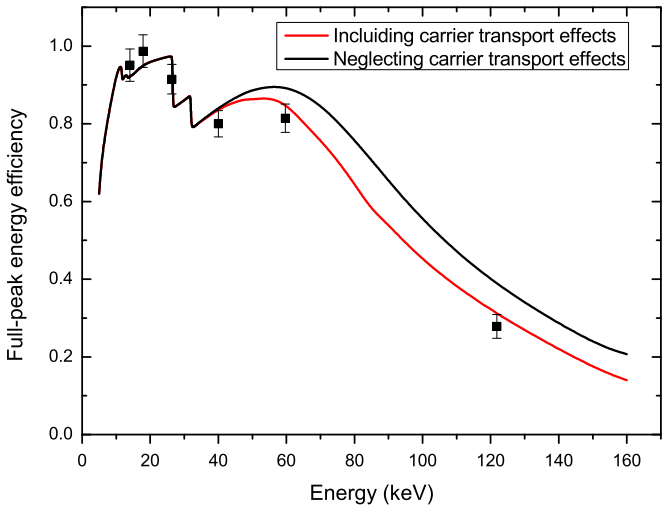

Fig. 3. Simulated and experimental full-energy peak efficiencies for the CdTe detector.

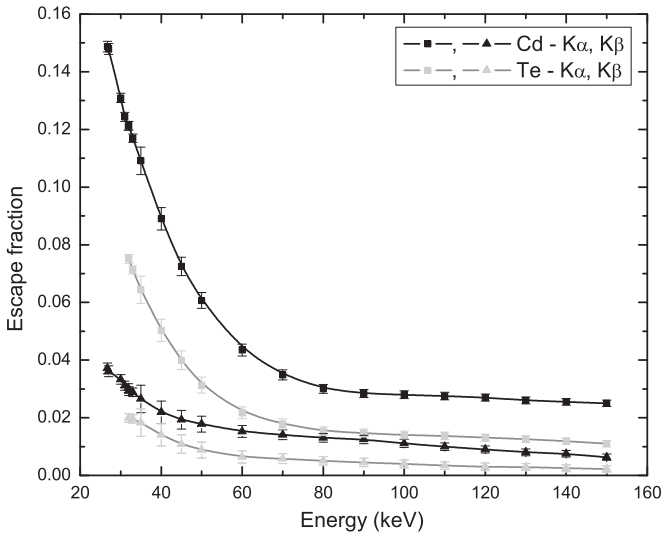

Fig. 4. Simulated escape fractions for the CdTe detector.

obtained with ^{241}Am and ^{152}Eu sources. Fig. 3 shows that both simulated full-energy peak efficiencies curves for the CdTe detector have a similar dependence with photon energy. The full-energy peak efficiency is maximum for energies between 10 and 27 keV, but it presents edges at 26.7 keV and 31.8 keV (Miyajima, 2003), which are related to the K-edges of linear attenuation coefficient of Cd and Te, respectively. For energies below 10 keV, the efficiency of the CdTe detector decreases rapidly, due to the absorption of radiation in the Be window. Besides, for energies greater than 50 keV the full-energy peak efficiency decreases, being less than 60% for 100 keV and 20% for 160 keV. The differences between the efficiencies determined by including or neglecting the carrier transport effects are small (up to 1%) for energies lesser than approximately 40 keV. For energies greater than 40 keV, the efficiency is significantly reduced by including the carrier transport effects in the simulation. The efficiency decreases up to 50% as the carrier transport is considered, being this decrease related mainly to poor hole transport. Thus, spectral distortions due to efficiency of CdTe detector are very important for all energy range, being most pronounced for energies lesser than 10 keV and higher than 27 keV (Miyajima and Imagawa, 2002; Künzel et al., 2004; Tomal et al., 2012). The experimental values of full-peak energy efficiency obtained with ^{241}Am and ^{152}Eu sources agree very well with the simulated values that include the carrier transport effects. These results highlight the importance of a detailed modeling of the carrier trapping and charge reflection to achieve a more realistic description of the response function of CdTe detector.

The escape fraction of K-characteristic radiation for the CdTe detector, computed from the simulated response functions, is shown in Fig. 4 as a function of the incident energy. Fig. 4 shows that the escape fractions for the K_α peaks are greater than that for K_β peaks due to their greater emission probability (Di Castro et al., 1984). The escape fraction for the K- characteristic peaks of cadmium and tellurium decreases when the incident photon energy increases, which is explained mainly due to the decrease of the probability of photoelectric effect with increasing energy. As shown in Fig. 4, the spectral corrections due to escape of characteristic radiation for the CdTe detector should be taken into account for energies above 26.8 keV. Besides, the escape fractions become lower than 5% for energies above 80 keV, so that this effect produces smaller spectral distortions.

3.2. X-ray spectra

Fig. 5 compares the measured and corrected x-ray spectra obtained with the CdTe detector for (a) 50 kVp and (b) 100 kVp. The spectra were normalized to unit area. As shown in Fig. 5, the correction procedure removes the spectral distortions at different energy range due to different physical effects observed on the response functions. The importance of each effect (i.e., escape of characteristic x-ray and efficiency of carrier transport) was investigated from the suppression and inclusion of each one in the correction procedure. The correction procedure removes the counts at low energies (<15 keV and <20 keV for 50 kVp and 100 kVp, respectively) present in the measured spectra, which can be attributed mainly to the Cd and Te characteristic x-ray escape. 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 Fig. 5, the correction of measured x-ray spectra for the response functions of the CdTe detector is fundamental to obtain more realistic spectra.

Table 2 shows the comparison between the half-value layers (HVL) and homogeneity coefficients (HC) values obtained experimentally and derived from the x-ray spectra uncorrected and corrected by the detector response for different beam qualities. The uncertainties in the HVL and HC experimental values also are included in Table 2, being smaller than 7.4%. From the results presented in Table 2, it was observed that the experimental values of HVL and HC are closer to the ones computed from the corrected x-ray spectra (with differences up to 7%), while the ones computed from the uncorrected x-ray spectra are significantly different (up to 38%). In general, the largest differences are found for highest tube potential, where the corrections by the detector efficiency and carrier transport are more important. Although the differences between the quality parameters for low tube potentials are smaller, the shape of the corrected spectra changes considerably after the correction procedure. In summary, the results of Table 2 show the relevance of a proper correction of the measured spectra by the detector response in order to achieve a better description of the radiation field produced by an x-ray tube. Thus, these results can be used as a validation test for the spectra measurement and correction from the detector response.

Fig. 6 shows the comparison between the 100 kVp x-ray spectrum obtained in this work, after correction for the response function of the detector, compared with that generated by the SpekCalc software (Poludniowski et al., 2009). As shown in Fig. 6, a

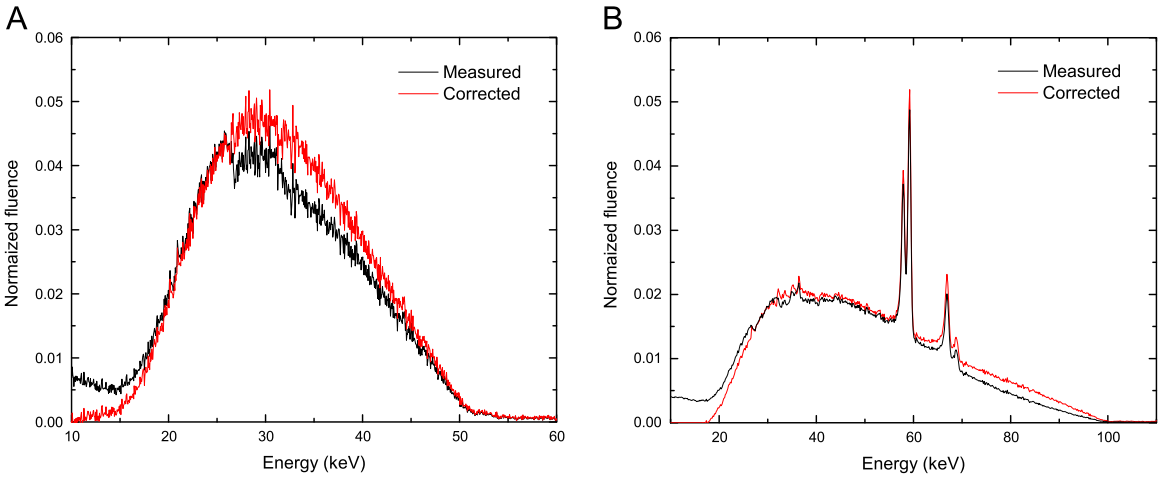

Fig. 5. Measured and corrected x-ray spectra obtained with CdTe detectors for (a) 50 kVp and (b) 100 kVp.

good agreement between the spectrum obtained in this work and the SpekCalc model is observed. The differences in the average energy were approximately 4% compared with SpekCalc (Poludniowski et al., 2009).

These results show the importance of the detailed knowledge of the response function and a proper correction procedure in order to achieve accurate x-ray spectra. The application of measured x-ray spectra using semiconductor detectors without a proper correction procedure could provide significant errors in the estimation of quality parameters of the beam and also in the determination of quantities used to study image quality and dose.

4. Conclusions

The results obtained in this and previous works show that the code PENELOPE modified to include specific features of the detector (i.e., carrier transport and energy resolution) can be a useful tool to determine the energy response functions of a semiconductor detector, with a good agreement with experimental data obtained using radioactive sources. The simulated response functions of the CdTe detector are significantly affected by the incident energy. The contribution of escape peaks to the total response is up 20% for low energies and decreases as the photon energy increases. At higher energies, the contribution of the carrier transport becomes more relevant, which is related to a decrease in the detector efficiency.

The present results for a CdTe detector showed that the shape of the x-ray spectra is significantly altered by the correction by the detector response through the stripping procedure. The measured spectra are in good agreement with those provided by a theoretical model from the literature. Besides, our results showed that HVL values computed from the corrected spectra are closer to the experimental ones, while the ones computed from the uncorrected x-ray spectra differ up to 27% of the experimental data. Thus, our results showed that the detailed knowledge of the response function and a proper correction procedure are fundamental to achieve more accurate spectra from which quality parameters can be extracted.

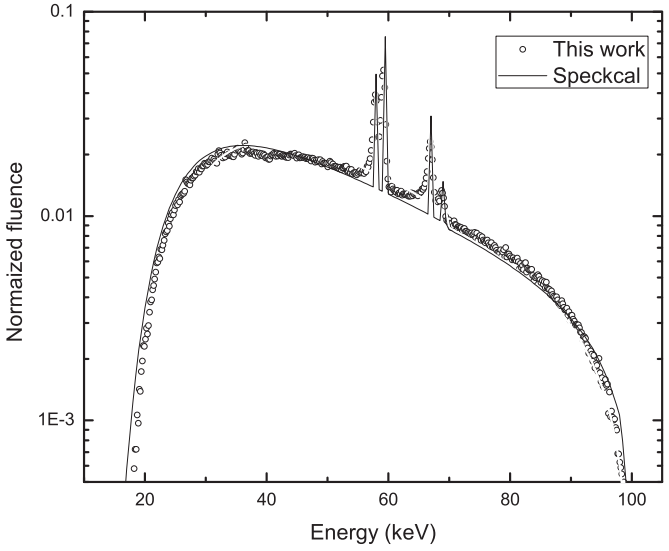

Fig. 6. Spectrum obtained for 100 kVp, compared with SpekCalc software (Poludniowski et al., 2009).

Acknowledgments

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Table 2
Beam quality parameters: experimental and computed from uncorrected and corrected x-ray spectra.

Beam quality	Tube potential (kV)	Added filtration (mm Al)	Experimental		Uncorrected spectra[a]		Corrected spectra[b]	
			HVL (mm Al)	HC	HVL (mm Al)	HC	HVL (mm Al)	HC
RQR 3	50	2.94	2.0 (1)	0.77 (1)	1.57	0.68	2.02	0.76
RQR 5	70	3.04	2.7 (1)	0.71 (2)	1.96	0.60	2.76	0.72
RQR 8	100	3.74	4.2 (2)	0.68 (2)	3.01	0.54	4.53	0.68
RQR 10	150	4.71	6.8 (5)	0.7 (2)	4.22	0.56	6.96	0.72

[a] Computed from the uncorrected spectra.
[b] Computed from the corrected spectra.

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