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Monte Carlo and least-squares methods applied in unfolding of X-ray spectra measured with cadmium telluride detectors

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Abstract

Spectra of calibration sources and X-ray beams were measured with a cadmium telluride (CdTe) detector. The response function of the detector was simulated using the GEANT4 Monte Carlo toolkit. Trapping of charge carriers were taken into account using the Hecht equation in the active zone of the CdTe crystal associated with a continuous function to produce drop of charge collection efficiency near the metallic contacts and borders. The rise time discrimination is approximated by a cut in the depth of the interaction relative to cathode and corrections that depend on the pulse amplitude. The least-squares method with truncation was employed to unfold X-ray spectra typically used in medical diagnostics and the results were compared with reference data.

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1. Introduction

The employment of cadmium telluride (CdTe) detectors is increasing in applications where portability is required. Compactness and portability are very attractive properties for using CdTe in characterization of X-ray beams commonly employed in medical applications, for example.

Characteristics of X-ray beams are usually obtained by unfolding the measured spectra, which requires the knowledge of the detector's response function. If the response function is well known, then the main source of errors in the reconstruction process would be the statistical errors of the measured spectrum. The stripping method [1,2] is commonly employed to reconstruct the original spectrum, although the propagation of errors for this procedure is not found in the literature. In this work, the least-squares method was employed in the unfolding of spectra measured with a CdTe detector and in the calculation of the associated covariance matrices of the reconstructed spectra. The response of the CdTe detector was simulated with the GEANT4 Monte Carlo toolkit [3], including a model for the charge collection efficiency. Simulated results were compared with experimental data obtained for standard calibration sources and X-ray beams.

2. The problem of spectrum unfolding

The detected spectrum, represented by a vector $\mathbf{d} = d_1, d_2, \ldots, d_n$, is related to the discrete spectrum of the sources of radiation $\mathbf{s} = s_1, s_2, \ldots, s_m$ through the expression

$$\mathbf{d} = \mathbf{R}\mathbf{s} \tag{1}$$

where $\mathbf{R}$ is a matrix that represents the response function of the instrument [4]. In the commonly employed method to obtain $\mathbf{s}$, called stripping method [1], the original spectrum is reconstructed from the largest to the smallest energies by applying the algorithm

$$s_i = \left[d_i - \sum_{j=i+1}^{m} R_{i,j} s_j \right] R_{i,i}^{-1}. \tag{2}$$

The propagation of experimental errors using this procedure is not found in the literature.

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Instead of the stripping method, in this study the least squares method was employed to obtain an estimate $\mathbf{s}'$ of the original spectrum

$$\mathbf{s}' = (\mathbf{R}^t\mathbf{V}_\mathbf{d}^{-1}\mathbf{R})^{-1}\mathbf{R}^t\mathbf{V}_\mathbf{d}^{-1}\mathbf{d} \quad (3)$$

and its covariance matrix, $\mathbf{V}_{\mathbf{s}'}$, given by

$$\mathbf{V}_{\mathbf{s}'} = (\mathbf{R}^t\mathbf{V}_\mathbf{d}^{-1}\mathbf{R})^{-1} \quad (4)$$

where the covariance matrix of $\mathbf{d}$, $\mathbf{V}_\mathbf{d}$, is diagonal with elements $\mathbf{V}_{\mathbf{d}i,i} = \sigma_i^2 = d_i$.

It is known from the theory of inverse problems that the solution of Eq. (3) presents huge oscillations and, in several cases, the inversion procedure is impossible due to singular matrix. For this class of ill-posed problem, regularization or truncation ($m<n$) methods [4,5] are applied to obtain a solution and eventually attenuate the oscillations.

The matrix $\mathbf{V}_{\mathbf{s}'}$ is necessary for the propagation of errors in any operation that involves $\mathbf{s}'$, as for example in the calculation of the mean energy of the unfolded spectrum. Defining the vector $\mathbf{e} = e_1, e_2, \ldots, e_m$, where e_i corresponds to the energy of the channel i, the mean energy is calculated by

$$\langle E\rangle = \mathbf{e}^t\mathbf{s}'A^{-1} \quad (5)$$

and its variance is obtained through

$$\sigma^2_{\langle E\rangle} = \mathbf{V}_{\langle E\rangle} = \mathbf{e}^t\mathbf{V}_{\mathbf{s}'}\mathbf{e}A^{-2} \quad (6)$$

where A is the sum of all elements of $\mathbf{s}'$.

3. The detector's response

The CdTe detector used in this study was made by Amptek (model: XR-100T-CdTe). This detector has a crystal with area of 3 mm^2 and thickness of 1 mm, operates at bias of 400 V, and has beryllium window with thickness of 250 μm. Additional information relevant for the detector modeling were taken from Amptek's documentation [6].

CdTe detectors exhibit spectral distortions mainly because of hole trapping, whose main effect is the presence of tails at the low-energy side of the full absorption peaks. The data acquisition system of XR-100T-CdTe includes the option of rise time discrimination (RTD). When operating with RTD, the slow rise time pulses are rejected and the low-energy tails are suppressed [7].

The detector's response function was calculated using the GEANT4 Monte Carlo toolkit [4] version 8.0.p01. For each interaction inside the CdTe crystal, two quantities were extracted: the deposited energy and the interaction position. Using this information, the charge collection efficiency can be calculated with the Hecht equation [8]

$$\eta(x) = [\lambda_h(1 - e^{-x/\lambda_h}) + \lambda_e(1 - e^{-(D-x)/\lambda_e})]D^{-1} \quad (7)$$

where D is the crystal thickness, x is the distance of the interaction position to the cathode, λ_h and λ_e are the drift length for holes and electrons, whose values (0.36 and 24 cm, respectively) were determined from measured spectra of ^{133}Ba, ^{241}Am and ^{152}Eu without RTD.

Fig. 1 shows ^{133}Ba spectra measured with and without collimation and RTD. The effect of RTD is evident from the tail suppression at the low-energy side of the full-energy peaks. After including a collimator, one observes suppression of background and lowering of a step-shaped structure at the low-energy peaks. Simulations including the collimator showed that this structure has large contribution from interactions that occur at the borders of the CdTe crystal. Comparison between simulated and experimental data, showed that the intensities of the low-energy photopeaks could be reproduced only after the inclusion of a dead layer near the cathode.

The best agreement between simulated and experimental data was achieved by calculating the charge collection efficiency with Eq. (7) for almost the whole crystal, but applying a continuous cut to represent dead layers in the regions near the cathode and the borders of the CdTe crystal. Complementary error functions were combined with the Hecht equation to produce continuous drop of the charge collection efficiency at the periphery of the detector: $f_i(t) = 0.5\{\mathrm{erfc}[(t-t_{ci})\alpha_i/l_i]\}$, where t_{ci} is the middle point of the dead layer corresponding to the coordinate t, l_i is the thickness of the dead layer and α_i is a parameter associated with the inclination of the curve at the cut position. Thicknesses of dead layers were 15 and 20 μm for cathode and borders, respectively. Electronic noise (120 eV) and statistical fluctuations (Fano factor = 0.1) were included as a Gaussian dispersion in the detector's response function.

Since the holes are slower than electrons, the principal effect of RTD is the rejection of slow pulses generated beyond a certain distance from the cathode [6]. Comparison between simulated and experimental spectra of ^{241}Am, ^{133}Ba and ^{152}Eu revealed that rejecting events generated at depths beyond 140 μm from the cathode is adequate to describe the efficiency up to 60 keV. The non-linear behavior of the employed RTD method, which shows dependence on the pulse amplitude, was taken into account

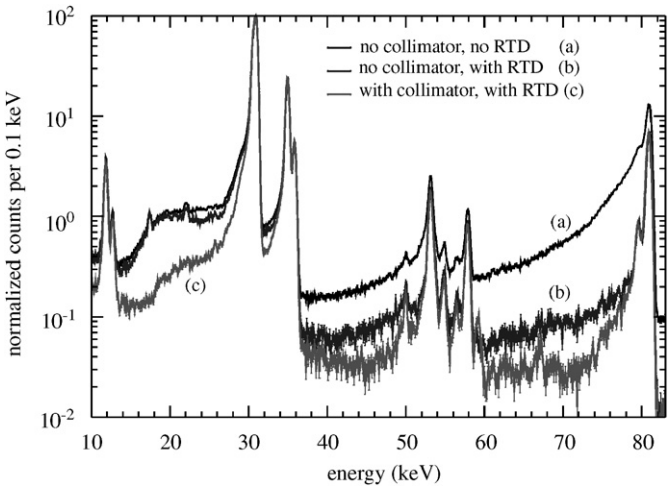

Fig. 1. ^{133}Ba spectra measured with a CdTe detector using different configurations.

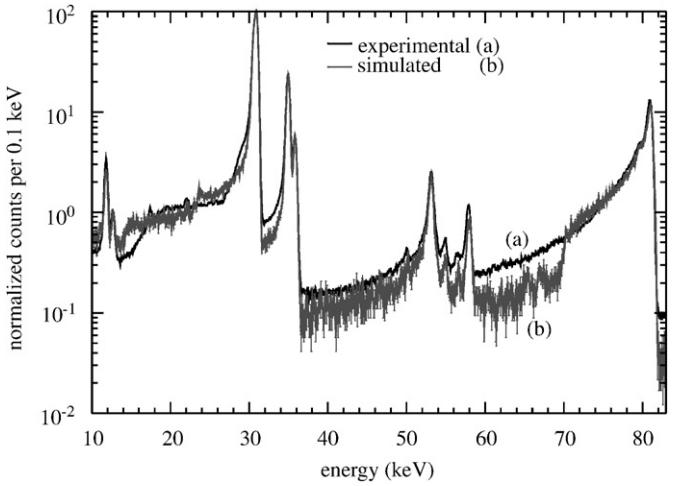

Fig. 2. ^{133}Ba spectrum measured with a CdTe without RTD and corresponding simulated spectrum.

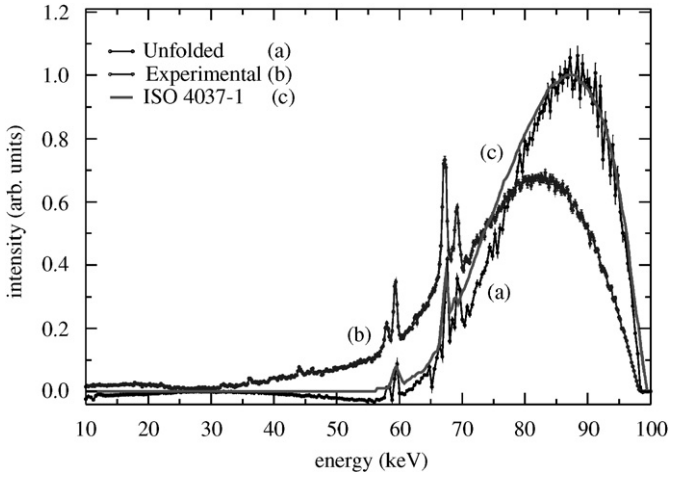

Fig. 3. Measured, unfolded and reference spectra of the X-ray beam with radiation quality N-100 [10].

by applying a correction to events with full-absorption energy greater than 60 keV.

4. Results

Experimental and simulated spectra of ^{133}Ba measured without RTD are shown in Fig. 2. The simulated spectrum reasonably reproduces tails, escape peaks and relative intensities of the measured spectrum. The background intensity and some small structures over the tails are not well described by the simulation. We believe that these discrepancies are due to imperfections in the active layer of the CdTe crystal, which were not taken into account in the simulation. Similar results were obtained for simulations with RTD and collimation.

Simulations of the detector's response function were performed for monochromatic photons from 5 to 155 keV in steps of 0.2 keV. The measured spectra were relocated to bins of 0.2 keV using the method described in Ref. [9].

Table 1
Mean energy and half value layers (HVL) of N-30 and N-100 radiation qualities beams [10] and calculated from unfolded spectra

Radiation quality	Quantity	ISO [10]	Unfolded
N-30	mean energy (keV)	24	25.71 (3)
	1st HVL (mm Al)	1.15	1.13 (2)
	2nd HVL (mm Al)	1.30	1.35 (3)
N-100	mean energy (keV)	83	85.22 (12)
	1st HVL (mm Cu)	1.11	1.03 (2)
	2nd HVL (mm Cu)	1.17	1.17 (3)

In parenthesis: errors with statistical origin.

The unfolding procedure with truncation ($n = 2\,\mathrm{m}$) was applied to produce the unfolded spectra in steps of 0.4 keV. Measurements of the radiation qualities N-30 and N-100 of the ISO narrow-spectrum series [10] were performed with collimator and RTD. The measured and unfolded spectra of quality N-100 are shown in Fig. 3. The unfolded spectrum presents small fraction of negative contributions at low energies, which are due to the imperfect modeling of the response function. Table 1 presents the mean energy and half-value layer of the unfolded spectra compared with reference values [10]. The difference between the reference and calculated values are greater than the statistical errors, which indicates that the model of the response function must be improved to represent the detector's response more realistically.

5. Conclusions

The least-squares method was applied to the discrete unfolding of X-ray spectra measured with a CdTe detector. The detector's response function was modeled with Monte Carlo simulations, using the GEANT4 toolkit, including effects of incomplete charge collection.

Comparison with reference spectra shows that the method produces satisfactory results to characterize X-ray spectra typically used in medical diagnostics. However, small differences between simulated and experimental spectra of standard sources show that the model used for the transport of charge carriers inside the CdTe crystal must be improved.

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