Response of CdZnTe Detector
in Measurement of Diagnostic X-ray Spectra

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Abstract
We calculated the response functions of a CdZnTe detector to be employed in x-ray spectrometry using LSCAT (Low energy photon SCATtering expansion for the EGS4 code). Incident energy of x-rays was from 10 to 150keV. In the usercode, the Hecht equation was utilized to deal with the effects of trapping of charge carriers in a CZT crystal. Parameters in the Hecht equation, the mean free path of charge carriers, were determined by comparing shapes of the peaks in the response functions with the ones in measured γ-ray spectra (source: ^{241}Am, ^{133}Ba). Finally, we corrected the measured x-ray spectra with the response functions. The results indicated a CdZnTe detector is valid as a x-ray spectrometer with proper corrections.

1 Introduction

X-ray spectrometry is the measurement of energy distribution in x-rays emitted from an x-ray tube. A High-Purity Germanium (HPGe) detector has usually been employed for its high efficiency and excellent charge transport properties[1]. In x- or gamma-ray spectrometry, output pulse height is not always proportional to the incident energy of x-rays because of escapes of the incident and secondary x-rays. Therefore, corrections for detector response are required to obtain a real x-ray spectrum; we need to calculate the incident x-ray energies from the output of a detector; the output indicates energy deposited by the incident x-rays. To do this, response functions of a detector are usually utilized to calculate a real x-ray spectrum from an output pulse height spectrum.

We employed a CdZnTe (CZT) detector as an x-ray spectrometer in this study. The CZT detector can be operated at room temparature because it has a large band gap. As a result, the detector doesn't need to be cooled by liquid nitrogen during measurement. It means a specroscopy system with a CZT detector is relatively compact. However, charge transport properties in the CZT crystal are poor because trapping of charge carriers is severe. For that reason, the effects should be corrected in addtion to the escape of incident and secondary x-rays.

In this study we analized a response of a CZT detector to monoenergetic x-rays to obtain parameters in corrections. We calculated response functions with the parameters. To validate the response functions, we corrected gamma-ray spectra and compared the results with the gamma-ray emission rate of source. After that, we corrected x-ray spectra using the response functions.

2 Methods

A CdZnTe crystal in the detector (Amptek XR-100T) was a density of 5.86g/cm^3 and atomic percentages of 45.0% (Cd), 5.0% (Zn), 50.0% (Te) respectively. The size was 3×3mm^2 with a thickness of 2mm. It had a 0.25mm Be window on its face. Bias voltage was 2500V/cm (500V/0.2cm). Incident x-rays were in pencil beams in both calculation and measurement.

2.1 Monte Carlo calculation

We calculated response functions of a CZT detector to monoenergetic x-rays with LSCAT (Low energy photon SCATtering expansion for the EGS4 code)[2]. Incident energy of x-rays was from 10 to 150keV in 0.5keV increments. The followings were especially taken into account in the code;

1. production of K-shell fluorescence x-rays (K x-rays),

2. effects of trapping of charge carriers.

Escape peaks of K x-rays in a spectrum are prominent for low energy x-rays such as diagnostic x-rays because the photoelectric effect is the most probable and the interactions tend to occur near a detector surface. However, the default version of EGS4 deals with production of K x-rays in elements. Therefore, we employed the test version of LSCAT (Low energy photon SCATtering expansion for the EGS4 code), which had been developed at KEK, to deal with K x-rays in compounds. Now the default version of LSCAT (`kek_improve`) can handle them easily[3].

Such semiconductors as CZT have poor charge transport properties because of their relatively high density of trapping centers. Since they cause incomplete charge collection, peaks in a spectrum have tails to the low energy side. Accordingly, we utilized the Hecht equation to take effects of them into account in the code.

$$\eta = \frac{\lambda_e}{D}(1 - \exp(\frac{-(D-x)}{\lambda_e})) + \frac{\lambda_h}{D}(1 - \exp(\frac{-x}{\lambda_h})) \tag{1}$$

where

η :ratio of induced charge to initial charge,

x :distance from interaction site to cathode,

D :thickness of a crystal,

λ_e :mean free path of electrons,

λ_h :mean free path of holes.

In this case, the induced charge due to energy deposition by an x-ray is equal to the initial charge multiplied by η. The parameters in the Hecht equation, mean free path of charge carriers, were determined by comparing shapes of peaks (tails) in response functions with the ones in measured gamma-ray spectra. And we determined the mean free path of electrons (λ_e) was 200 times larger than that of holes (λ_h) in reference to literature on this subject to reduce the parameters in Monte Carlo calculations, i.e. the parameter in the calculation was λ_h only.

In the code, cut off energy was set at 5.0keV for photons (`AP=0.005` in the PEGS4 input file) and 150.0keV for electrons (`ECUT=0.150+0.511` in the EGS4 user code; we did not transport electrons). To consider the electron binding effects in the Rayleigh and Compton scattering, options in the PEGS4 input files and the EGS4 user code were turned on (`IRAYL=1, IBOUND=1, INCOH=1` in the PEGS4 input files, `IRAYLR(I)=1, INCOHR(I)=1` in the EGS4 user code).

2.2 Experimental considerations

In measurement, we placed collimators in front of the detector (0.8mmϕ for gamma-rays, 0.4mmϕ for x-rays, made from tungsten). We usually use collimators in x-ray spectrometry to reduce pulse pileup. The pulse pileup causes distortion of the output spectrum which cannot be easily corrected. Channel width was 0.1keV per channel in gamma-ray spectrometry and 0.5keV per channel in x-ray spectrometry. The channel width for gamma-rays was smaller to avoid distortion due to the channel width; after FWHM (Full Width at Half Maximum) analysis, the gamma-ray data was converted to data of 0.5keV per channel for correction procedures.

To compare measured peaks in gamma-ray spectra with the ones in response functions, we have to remove distortion due to electric noise and statistical fluctuations in number of charge carriers because the response functions don't contain these effects. Therefore, we employed the unfolding method to calculate a spectrum without this distortion. In the procedure, we regarded effects of this distortion as gaussian distribution based on measured FWHM. In the unfolding method, we used relations between input and output as follows.

$$M(E) = \int_0^\infty R(E, E')S(E')dE' \tag{2}$$

where

$S(E')$:number of input x-rays with energy E',

$R(E, E')$:response functions (matrix); probability of detection in channels corresponding to energy E with incident energy E',

$M(E)$:number of output x-rays counted in channels corresponding to energy E.

We can obtain the input $(S(E))$ by solving the determinant(2). This determinant can be solved as simultaneous equations.

2.3   Correction for spectra

We employed the stripping method to correct gamma- and x-ray spectra[4-6]. In the stripping method, we assume counts in each channel consist of the following two components;

1. counts due to photoelectric effect without trapping,

2. counts due to contribution by incident x-rays with higher energies going through escapes of secondary x-rays or trapping of charge carriers during charge transport.

In energy deposition in 2nd case, x-rays are counted on channels lower than the incident energy. Procedures of the stripping method are as follows;

1. remove counts due to 2. in spectrum,

2. divide the counts to be left with probability of full energy deposition without trapping (1.).

This procedure is represented by the following equation.

$$S(E) = \frac{M(E) - \sum_{E'=E+1}^{E_{max}} R(E, E')S(E')}{R(E, E')} \tag{3}$$

where

$S(E)$:number of incident photons with energy E,

$M(E)$:number of output photons counted in channels corresponding to energy E,

E_{max} :maximum energy of a x-ray spectrum (determined by tube voltage),

$R(E, E')$:response functions; probability of detection in channels corresponding to energy E with incident energy E'.

In this procedure, we assume counts in the highest energy of x-ray spectra don't contain counts due to contribution from its higher energies, i.e. the $M(E_{max})$ is equal to the $S(E_{max})$.

2.4 Evaluation of results

First, to validate the calculated response functions, we corrected gamma-ray spectra of ^{241}Am using them and compared relative intensity of peaks in corrected spectra with the gamma-ray emission rate of ^{241}Am. If the response functions are valid, corrected results are close to input data, i.e. source data of Radio Isotopes. Next, we corrected measured x-ray spectra with the response functions. The results were compared with corrected spectra measured with a HPGe detector.

3 Results

The results we obtained in this study were as follows;

1. In the response functions calculated with the code, escape peaks of each element (Cd, Zn, Te) and tails of each peak appeared (Fig.1). Parameters in the calculations were $\lambda_h = 0.20cm$ ($\mu\tau_h = 8.010^{-5}cm^2/V$ in $2500V/cm$), $\lambda_e = 40.0cm$ ($\mu\tau_e = 1.610^{-2}cm^2/V$ in $2500V/cm$).

2. In gamma-ray spectra corrected with the response functions, relative counts of peaks were in good agreement with the gamma-ray emission rate of source. At the same time, tails to the low energy side of the peaks, due to trapping of charge carriers, also disappeared in spectra (Fig.2). The results meant input spectra were calculated from output spectra and the response functions were valid.

3. X-ray spectra corrected with the response functions were close to corrected spectra measured with a HPGe detector (Fig.3).

4 Discussions

As you can see in Fig.4, tails in the response functions don't completely fit the ones in measured gamma-ray spectra. The discrepancies were more significant in the high energy region. We suppose there are problems in the assumptions made in the Hecht equation. In the Hecht equation, the followings are assumed;

1. trapped charges are not detrapped,

2. a uniform density of trapping centers in a crystal exists,

3. electric field in a crystal is uniform.

Since presence of detrapping in a CZT crystal and models including the effects are already published, we should take the effects into account in the code.

And the discrepancies in the high energy region of x-ray spectra must also be due to differences between calculated and measured responses. We believe the discrepancies must be smaller with improvements made on the model related to the trapping of charge carriers.

5 Conclusions

We calculated response functions of a CdZnTe detector using LSCAT (Low energy photon SCATtering expansion for the EGS4 code). Corrected spectra with the response functions were close to the ones measured with a High Purity Germanium detector. A CdZnTe detector can be used in x-ray spectrometry with proper corrections.

References

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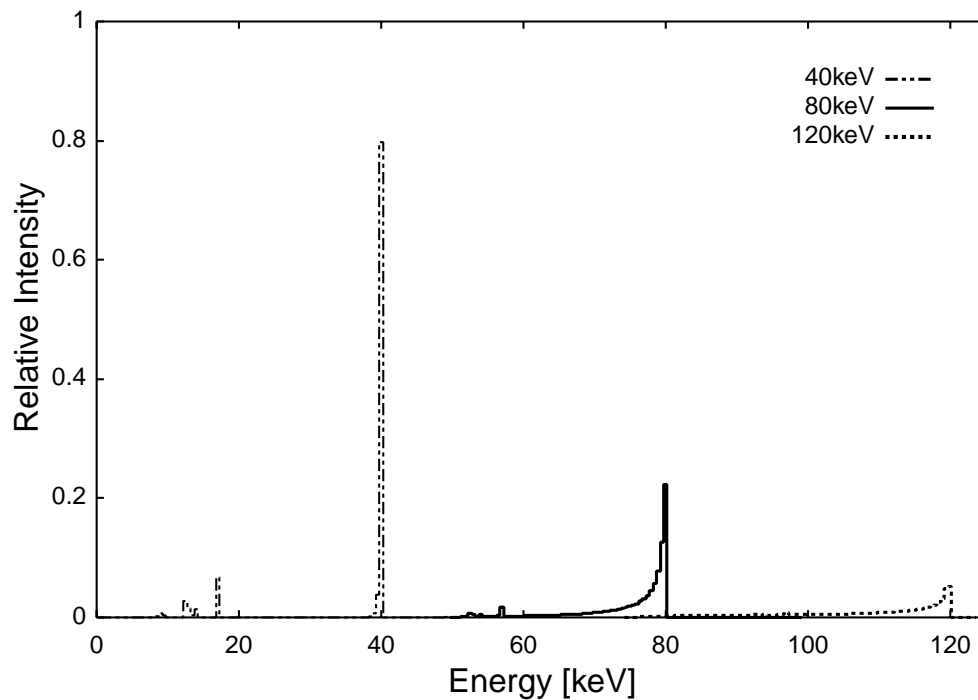
Figure 1: Response functions calculated with EGS4. Incident energy of x-rays are 40keV, 80keV and 120keV respectively.
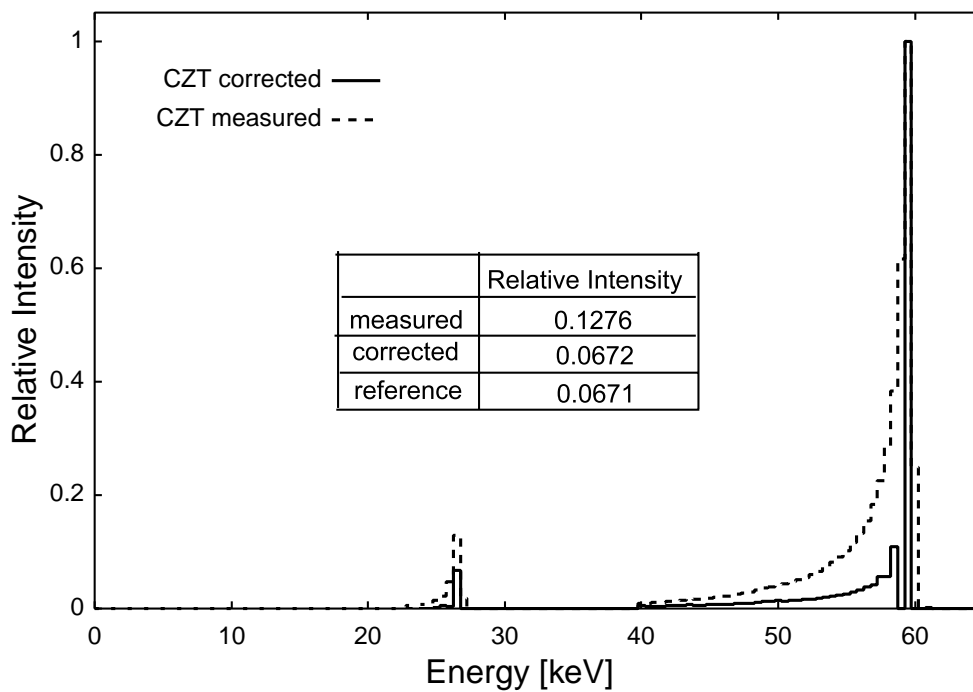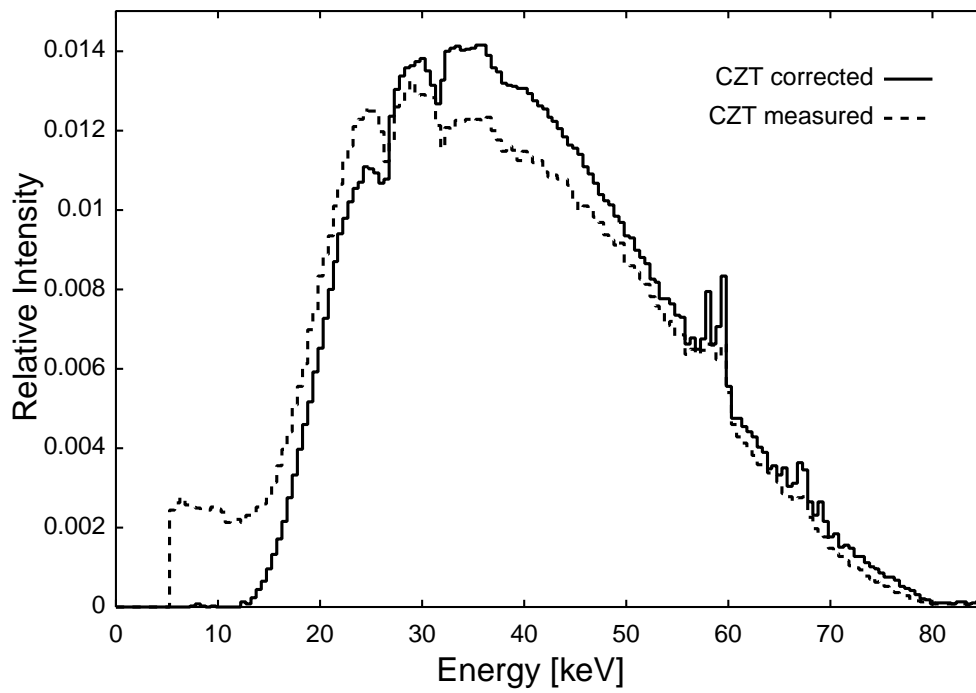
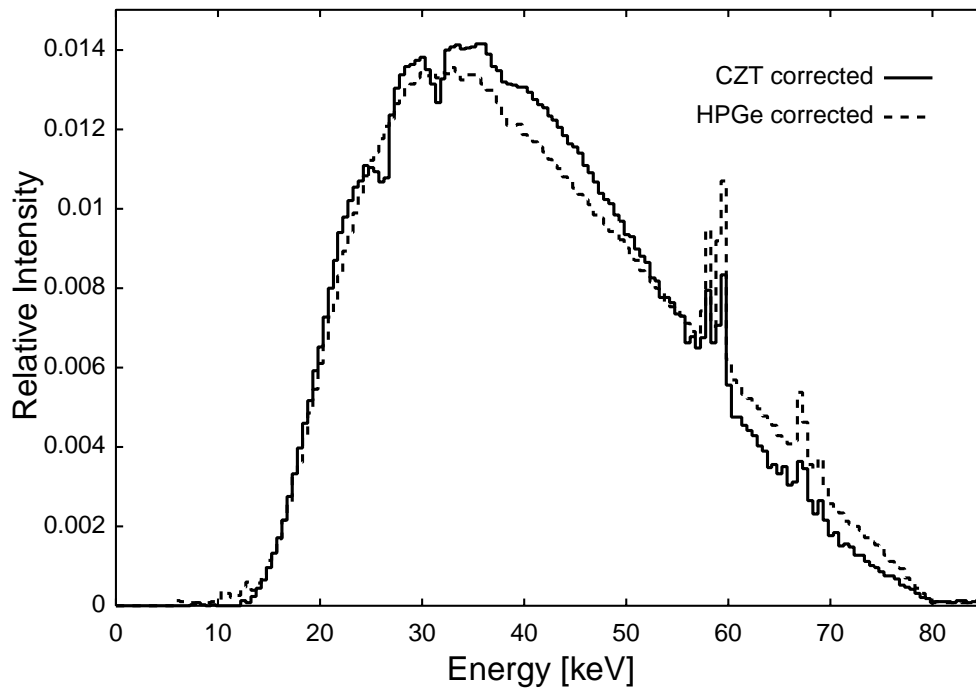|	Relative Intensity
measured	0.1276
corrected	0.0672
reference	0.0671

Figure 2: A corrected gamma-ray spectrum compared with the measured one. Source was ^{241}Am. Tails of peaks disapeared and relative intensity of peaks (26.3/59.5keV) agree well with gamma-ray emission rate of source.

Figure 3: (a) A corrected x-ray spectrum compared with the measured one. Tube voltage was 80kV. In the corrected spectrum, low energy components are less than the ones in the measured spectrum.
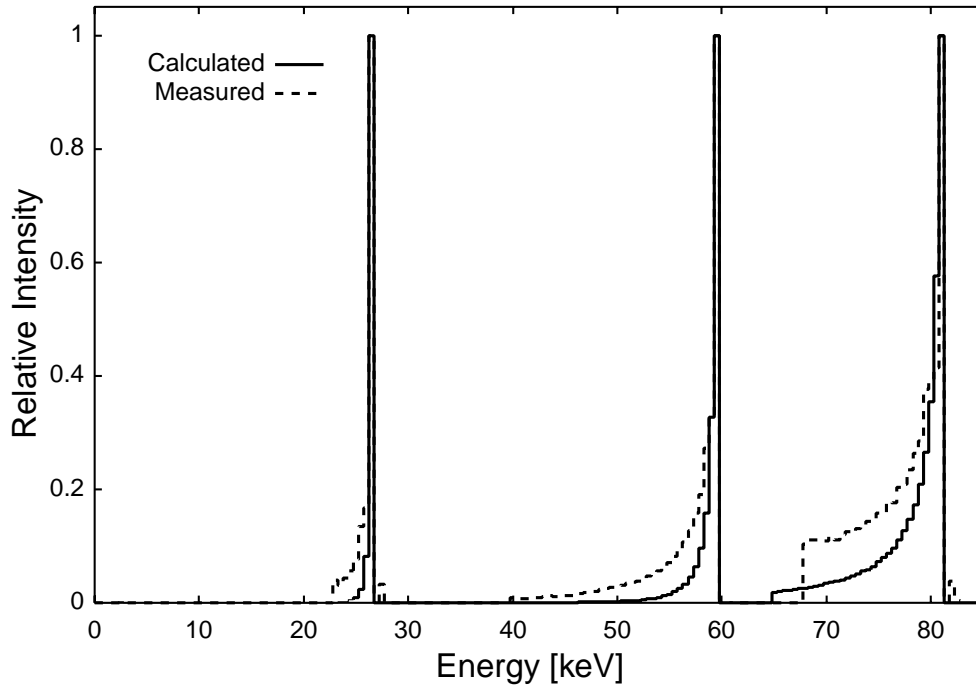(b) A corrected x-ray spectrum compared with a HPGe detectore. Tube voltage was 80kV.

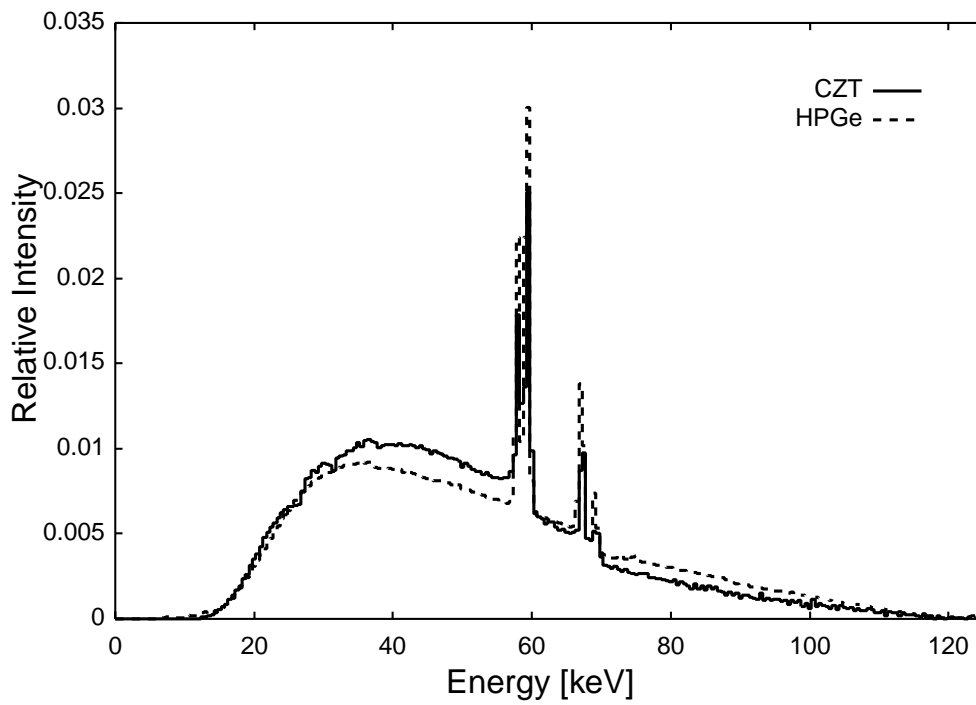Figure 4: Difference in tails between measured and calculated data.

Figure 5: A corrected x-ray spectrum. Tube voltage was 120kV.