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K-edge energy-based calibration method for photon counting detectors

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Abstract

In recent years, potential applications of energy-resolved photon counting detectors (PCDs) in the x-ray medical imaging field have been actively investigated. Unlike conventional x-ray energy integration detectors, PCDs count the number of incident x-ray photons within certain energy windows. For PCDs, the interactions between x-ray photons and photoconductor generate electronic voltage pulse signals. The pulse height of each signal is proportional to the energy of the incident photons. By comparing the pulse height with the preset energy threshold values, x-ray photons with specific energies are recorded and sorted into different energy bins. To quantitatively understand the meaning of the energy threshold values, and thus to assign an absolute energy value to each energy bin, energy calibration is needed to establish the quantitative relationship between the threshold values and the corresponding effective photon energies. In practice, the energy calibration is not always easy, due to the lack of well-calibrated energy references for the working energy range of the PCDs. In this paper, a new method was developed to use the precise knowledge of the characteristic K-edge energy of materials to perform energy calibration. The proposed method was demonstrated using experimental data acquired from three K-edge materials (viz., iodine, gadolinium, and gold) on two different PCDs (Hydra and Flite, XCounter, Sweden). Finally, the proposed energy calibration method was further validated using a radioactive isotope (Am-241) with a known decay energy spectrum.

1. Introduction

In the past decade or so, energy-resolved x-ray photon counting detectors (PCDs) have attracted a lot of research interest due to their unique ability to reject electronic noise and the potential to enable x-ray spectral imaging. As a matter of fact, the applications of PCDs have motivated several innovative x-ray imaging methods in both clinical and biological fields. For example, PCDs allow detected x-ray photons to be sorted into different energy bins. As a result, material decompositions can be performed to achieve spectral CT imaging (Wang et al. 2011, Lakshmanan et al. 2016, Yu et al. 2016). Imaging can also be performed using

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energy bins below and above material K-edge energy to significantly boost contrast in K-edge imaging (Schlomka et al. 2008, Feuerlein et al. 2008, Roessl et al. 2011, Sato et al. 2012, Rink et al. 2013). When PCD imaging capabilities are combined with one or more contrast agents (Schlomka et al. 2008, Lakshmanan et al. 2016), molecular CT imaging methods may be developed for personalized medicine (Taguchi & Iwanczyk 2013). In addition, recent studies have also demonstrated that the energy-resolving capability of PCDs may be utilized to improve the imaging performance for the grating-based x-ray differential phase contrast imaging (Pelzer et al. 2013, Thuring et al. 2013, Ge et al. 2016).

In conventional energy-integration x-ray detectors, the deposited photon energy is integrated to generate signals. In contrast, energy-resolved PCDs count the number of incident x-ray photons with certain energies (Llopart et al. 2002). In PCDs, x-ray photons first interact with the photoconductor to transfer energy to the ionized charges. These ionized charges are then collected, amplified, and shaped to generate electronic signals, i.e., voltage pulses. The pulse height is then compared with the preset energy threshold values using comparators to sort the incident x-ray photons into different energy bins. For a PCD equipped with the anti-charge sharing function (Ballabriga et al. 2007, Gimenez et al. 2011), the pulse height is proportional to the incident x-ray photon energy. However, the threshold values used in PCDs is not often calibrated to the absolute energy values by the vendors and thus arbitrary units (rather than the more meaningful effective x-ray photon energies) have been used as the energy thresholds. Consequently, when precise knowledge of photon energy is needed in specific applications, energy calibration must be performed to establish the quantitative relationship between the PCD energy threshold values and the corresponding absolute x-ray photon energy values.

To calibrate energy for PCDs, both mono-energetic and poly-energetic methods have been proposed. In the mono-energetic approach, an x-ray source to generate photons with well-calibrated energy is required. This can be achieved using either x-ray synchrotron beams or radioactive isotopes. In this regard, the synchrotron (Ponchut et al. 2002, Gimenez et al. 2011) is an ideal candidate for an energy calibration source, due to its adjustable beam energy with relatively high energy resolution. The high photon flux also enables short data acquisition time. However, given the limited access to synchrotron beam lines, it is not practical for general users to use this method to calibrate energy for their PCDs. Radioactive isotopes are another option for monoenergetic gamma-ray sources, but the available radioactive isotopes for the energy range between 20 keV to 140 keV are often limited and the data acquisition time can be long due to their low specific activities (Koenig et al. 2012, Guni et al. 2011). Methods utilizing x-ray fluorescence to calibrate PCDs (Ronaldson et al. 2011, Ballabriga et al. 2011, Talla 2011, Cho et al. 2014, Ding et al. 2014) have also been proposed. However, the detected x-ray fluorescence photons are inevitably contaminated by Compton scattering events with different energies. Therefore, the imaging geometry and detector position need to be carefully designed to reduce the confounding impact from scattered photons for successful calibration.

In addition to mono-energetic methods, methods utilizing poly-energetic x-ray beams have also been proposed to perform PCD energy calibration (Das et al. 2015, Panta et al. 2015, Lee et al. 2016). In this method, the x-ray tube potential kVp values are used to calibrate the

PCDs since the highest photon energy generated from an x-ray tube is determined by the tube potential. Therefore, in principle, one can adjust the energy threshold value to match the highest photon energy at a given tube potential such that there are no photons recorded beyond a certain threshold value. In this way, the corresponding relationship between the PCD threshold value and the photon energy can be established for several different tube potentials used to acquire data for energy calibration. However, in practice, this clever method encounters two major challenges: the fluctuations of tube potential and the non-uniform energy response from one detector element to another. As a result of these challenges, in practice it is very difficult to determine the energy threshold value that corresponds to the highest photon energy at a given tube potential and thus the performance of the method may be compromised.

In this paper, we propose an energy calibration method using the characteristic K-edge energy of materials. Due to the energy quantization of atomic electrons in an atom, the lowest energy required for photoelectric interaction for K-shell electrons is determined by the K-shell binding energy. When the K-shell binding energy falls within the range of a polychromatic x-ray spectrum, there is a discontinuity in energy dependence of x-ray absorption. This discontinuity is determined by the quantized K-shell binding energy and thus bears the name of K-edge energy. Although there are other edges such as L-edge and M-edge and so forth at energies lower than the K-edge energy, either these energies do not fall within the range of polychromatic x-ray spectrum or the contribution of these edges are small compared with other contributions with continuous energy dependence. As a result, the potential discontinuities in absorption at these edges are not as clearly visible as that at the K-edge (Attix 2008). Due to the discontinuity, there are two attenuation coefficient values for the same K-edge energy. If one wants to precisely measure the abrupt change of the attenuation coefficient curve, PCDs with δ -function like energy response. In practice, due to the limited energy resolution of a real PCD, the measured attenuation curve only demonstrates a smoothed local peak and a local valley. Therefore, the smoothed K-edge can be modeled as a convolution between the theoretical K-edge profile and the detector energy response function. In the following sections, the theoretical framework of the proposed method will be further elaborated, experimental measurements to demonstrate how this method can be used to perform energy calibration for PCDs will also be presented, and, finally, a radioisotope Am-241 will be used to further validate the proposed method.

2. Methods

2.1. Theoretical foundation

When a PCD with energy response function $\Gamma(E)$ is used to measure an energy dependent attenuation curve $\mu(E)$, the obtained attenuation curve $\mu_m(E)$ is a convolved result, provided that the energy response function of the PCD can be considered a shift-invariant function. This approximation is generally valid, as long as the energy range is relatively narrow. In the case under study, the energy window is restricted to a range centered around the K-edge energy of the material. Namely, the measured attenuation curve is modeled as:

$$\mu_m(E) = \mu(E) \otimes \Gamma(E). \quad (1)$$

In Eq. (1), $\mu_m(E)$ denotes the experimentally measured energy dependent K-edge attenuation curve, $\mu(E)$ is the theoretical material attenuation curve with K-edge response, and function $\Gamma(E)$ is the assumed shift-invariant energy response function of the PCD.

The energy response function $\Gamma(E)$ of a specific PCD may have complex structure with respect to energy (Roessler et al. 2011). However, in the neighbor of K-edge energy, the smearing of the K-edge attenuation curve by the finite energy resolution of the PCD can be modeled by a Gaussian kernel as follows:

$$\Gamma(E) = \frac{1}{\sqrt{2\pi\sigma_E^2}} \exp\left(-\frac{E^2}{2\sigma_E^2}\right). \quad (2)$$

In Eq. (2), σ_E quantifies the energy resolution of the PCD. A larger σ_E corresponds to decreased PCD energy resolution and vice versa.

To better understand how the σ_E parameter of the Gaussian kernel impacts the shape of the theoretical K-edge response function $\mu(E)$, numerical simulations were performed. As an example, iodine was used as the K-edge material (its K-edge energy $E_k = 33.2$ keV). The mass attenuation coefficients of iodine were obtained from the NIST (National Institute of Standards and Technology) database (Hubbell & Seltzer 1995) in the energy range between 15.0 keV to 60.0 keV. The available eight values of the mass attenuation coefficients were upsampled using the Lagrange interpolation method (denoted as Lagrange in figure 1). The upsampled mass attenuation curve is then convolved with the aforementioned Gaussian kernel with different σ_E to demonstrate the smearing of the K-edge by different energy response functions. Three different values of σ_E (i.e., 1.0 keV, 3.0 keV, and 8.0 keV) were studied and results were presented in figure 1. As one can observe from the results, when the value of σ_E increases, the discontinuous K-edge is smeared into one smoothed peak and one smoothed valley (referred to as the K-edge signature in this paper). When the response function is further widened, the K-edge signature may be completely lost in the measured mass attenuation curve. In the studied example, the K-edge signature is totally lost when $\sigma_E=8.0$ keV.

2.2. Data analyses method

As demonstrated in the numerical results in figure 1, the vertical jump in the theoretical attenuation curve at the K-edge energy E_k may be smeared into two extrema: one local minimum (valley) and one local maximum (peak), when a PCD with finite energy resolution is used to measure the curve. The corresponding energies of the local minimum and maximum are denoted as E_v and E_p respectively and they are different from the K-edge energy E_k . In fact, the K-edge energy E_k is always located between E_v and E_p , namely, $E_v <$

$E_k < E_p$. These three energy values correspond to three PCD threshold values T_v , T_k , and T_p . Obviously, they can be sorted into the following order: $T_v < T_k < T_p$.

From the experimentally measured valley-peak shaped attenuation curve $\mu_m(T)$, the PCD threshold values of T_v and T_p can be readily determined. However, the PCD threshold T_k that corresponds to the K-edge energy E_k is still difficult to determine. All we know is that T_k is located between T_v and T_p , but its precise location is unknown. In this paper, we make a conservative assumption that T_k has equal probability to appear in the range of $[T_v, T_p]$, namely, the probability density function is given by:

$$p(T_k) = \frac{1}{T_p - T_v}, T_k \in [T_v, T_p]. \quad (3)$$

Under this statistical assumption, the mean value of T_k can be estimated and expressed by

$$\hat{T}_k = \frac{T_v + T_p}{2}. \quad (4)$$

Additionally, the statistical error, i.e., standard deviation $\sigma_{\hat{T}_k}$, of T_k is given by

$$\sigma_{\hat{T}_k} = \frac{T_p - T_v}{2\sqrt{3}}. \quad (5)$$

Using the $\hat{T}_k$ and the already known K-edge energy E_k , the linear relationship between the detector threshold T and the photon energy E can be finally established. In this paper, the linear relationship is assumed to be:

$$\hat{T}_k = aE_k + b. \quad (6)$$

The variable $\hat{T}_k$ has units of detector threshold value, E_k has units of keV, coefficient a represents the slope, and coefficient b corresponds to the intercept. In principle, by measuring several different K-edge materials, one is able to determine the coefficients a and b and thus achieve the energy calibration for a given PCD.

In summary, the proposed energy calibration method was performed as follows:

- i. Find the threshold values T_v and T_p from the measured energy dependent attenuation curve of a certain K-edge material;
- ii. Determine $\hat{T}_k$ using Eq. (4);
- iii. Form data pair $(E_k, \hat{T}_k)$;

- iv. Use multiple pairs of data acquired from different K-edge materials to determine the linear regression coefficients a and b .

2.3. Experimental materials and methods

To demonstrate the feasibility of the proposed energy calibration method, experimental studies were performed on an x-ray benchtop imaging system. Two models of x-ray energy-resolved PCDs using CdTe photoconductors were calibrated: XC-Hydra FX50 (denoted as Hydra) and XC-Flite X1 (denoted as Flite). Both detectors are manufactured by XCounter AB in Sweden. The Hydra detector features an imaging area of $512.0 \text{ mm} \times 6.0 \text{ mm}$, while the Flite detector has an active area of $153.6 \text{ mm} \times 12.8 \text{ mm}$. The native detector element size of the two detectors was $100.0 \text{ } \mu\text{m} \times 100.0 \text{ } \mu\text{m}$. Both the Hydra and Flite detectors have two distinct energy thresholds and were operated with the anti-charge-sharing mode.

In experimental studies, three different K-edge materials were used: iodine, gadolinium, and gold. Their corresponding K-edge energies are 33.2 keV, 50.2 keV, and 80.7 keV, respectively. The iodine contrast agent (Omnipaque 300, GE Healthcare) and the gadolinium contrast agent (Magnevist, Bayer) used for medical imaging applications were imaged to generate the K-edge attenuation curves of the iodine and gadolinium materials. Specifically, each milliliter of iodine contrast agent contained 75 mg iodine, and each milliliter of gadolinium contrast agent contained 469 mg gadopentetate dimeglumine. The two liquid contrast agents were imaged in two PMMA containers, which had square cross sections with an inner dimension of $1.0 \text{ cm} \times 1.0 \text{ cm}$ and an outer dimension of $1.3 \text{ cm} \times 1.3 \text{ cm}$. To study the K-edge response of gold material, a $200 \text{ } \mu\text{m}$ thick gold absorber was used.

To measure the attenuation of a K-edge material at a threshold T , an energy window (i.e., $[T - \frac{\Delta T}{2}, T + \frac{\Delta T}{2}]$) with two thresholds $T - \frac{\Delta T}{2}$ and $T + \frac{\Delta T}{2}$ was used, where T denotes the center of the energy window and ΔT denotes the window width. The detector readings at these two thresholds with and without the object were measured. The attenuation at the threshold T was then determined using the following formula:

$$\mu(E)L = \ln \frac{I_0(T - \Delta T/2) - I_0(T + \Delta T/2)}{I(T - \Delta T/2) - I(T + \Delta T/2)}, \quad (7)$$

where $I_0(T \pm \Delta T/2)$ denotes the detector reading at threshold $T \pm \frac{\Delta T}{2}$ without the object (air scan) and $I(T \pm \frac{\Delta T}{2})$ denotes the detector reading at threshold $T \pm \frac{\Delta T}{2}$ with the object. The above process was repeated to measure the attenuation at different thresholds to obtain the attenuation curve. Table 1 lists the detailed experimental parameter settings of the two PCDs used in this paper.

The x-ray tube (model: Varian G1592) was operated at 50 kV, 80 kV, and 110 kV for the measurements of the iodine contrast agent, gadolinium contrast agent, and gold absorber, respectively. The x-ray beams were carefully filtered to make sure that the mean energy of each x-ray spectrum is centered around the K-edge energy of each material with a relatively

narrow distribution. This can be accomplished by selecting the appropriate tube potential for each K-edge material and with the added beam filter to filter out the low energy photons in the spectrum. The added beam filtrations for each x-ray beams are listed in table 2. Table 2 also includes other beam parameters and x-ray exposure parameters of the experiment. To reduce noise, the attenuation of an ROI containing 2500 pixels was averaged to represent the attenuation of a given energy window. From the experimentally measured attenuation curve, the peak and valley of the curve were directly identified from experimental data points and used in data analysis presented in the previous section.

2.4. Validation studies using radioactive isotope

To validate the energy calibration method and to check the accuracy of the proposed energy calibration strategy, an Am-241 isotope was used. The energy of the primary gamma emission of this isotope is 59.5 keV. The Am-241 isotope source had an activity of 10 μCi and was mounted directly on the detector surface. For the Hydra detector, the energy threshold unit was varied from 40.0 up to 120.0 with an incremental interval of 2.0. For the Flite detector, the energy threshold unit was changed from 2.5 to 18.5 with an interval of 0.5. From the experiment, one can determine the PCD threshold value T corresponding to the peak gamma energy. With the obtained linear relationship in Eq. (6), the experimentally measured peak gamma emission energy of Am-241 isotope can then be estimated and compared with the ground truth to determine the accuracy of the calibration method.

3. Results

3.1. PCD energy calibration results

Figure 2 presents the measured results for three different K-edge materials. As shown in these plots, the horizontal axes have the detector threshold unit, and the vertical axis denotes the line integral values ($\mu(E) \times \text{path length}$) of the K-edge material. As can be observed, the valley-peak structure (K-edge signature) is well maintained. From the experimental results, the location of the valley and peak for every K-edge material can be measured, and results are presented in table 3. In addition, the mean values of the detector threshold corresponding to the K-edge energy E_k and their experimental errors were also estimated using Eq. (4) and Eq. (5). Results are further listed in table 3.

Using the three measured $(E_k, \hat{T}_k)$ dataset, together with the already known K-edge energy values E_k , the linear relationship between the energy threshold T and the photon energy E was determined for the two different detectors, separately. Herein, the standard weighted linear regression was performed in Matlab (The MathWorks, Natick, MA). Results are plotted in figure 3. The energy calibration result was found to be

$$T = 1.85E - 6.78, \quad (8)$$

for the Hydra detector and

$$T = 0.29E - 2.08, \quad (9)$$

for the Flite detector.

3.2. Am-241 isotope validation results

Figure 4 shows the measured spectrum of the Am-241 isotope for both the Hydra and Flite detectors. Gaussian fittings were performed to estimate the central peak positions. According to the fittings, the peak center is 101.2 for Hydra, and 15.6 for Flite. Using the obtained energy calibration result in Eq. (8), the measured gamma photon energy of Am-241 isotope is found to be 58.2 keV, of which the 95% confidence interval is [53.6 keV, 63.4 keV], for the Hydra detector. Similarly, the measured energy of Am-241 isotope is found to be 61.3 keV, of which the 95% confidence interval is [57.3 keV, 65.7 keV], for the Flite detector. Essentially, the estimated gamma photon energy of Am-241 from the two detectors are very close to the native 59.5 keV gamma photon energy of Am-241 ($< 2.5\%$ experimental error for the Hydra detector, and $< 3.5\%$ experimental error for the Flite detector). Additionally, the 59.5 keV gamma photon energy of Am-241 falls within the predicted energy interval. These experimental results suggest that the accuracy of this newly developed energy calibration method is quite good.

4. Discussion

In this work, a new PCD energy calibration method using the material characteristic K-edge information has been proposed and experimentally validated. Compared with other PCD energy calibration methods, the proposed PCD calibration strategy has several advantages. First of all, the requirements on x-ray beam are flexible: neither mono-energetic x-ray beams, nor radioactive isotope sources and special x-ray filtration materials are required. Second, this method is immune to the tube voltage fluctuations. Third, the K-edge materials are fairly easy to prepare, particularly for laboratories conducting medical imaging research. Finally, the experimental imaging setup such as the imaging geometry, is easy to implement in the laboratory environment.

Despite the potential advantages of the proposed PCD energy calibration method, it does have some potential limitations. First of all, when the energy resolution of the detector is too poor (as shown in figure 1 for $\sigma_E = 8$ keV), the K-edge signature in the measured attenuation curve may be completely smeared and thus the required peak and valley values to estimate the corresponding threshold value $\hat{T}_k$ at K-edge energy may not be found. As a result, this proposed method may become invalid to calibrate PCDs. Note that the anti-charge sharing functionality in PCDs may help improve detector energy resolution. In the results presented in this paper, the available anti-charge sharing function was turned on. It remains to be investigated how the anti-charge sharing function may impact the proposed energy calibration method and the calibration results since the change of the calibration results may become an indicator of potential energy resolution change with and without the anti-charge sharing function. Another cause of energy resolution degradation is the pulse pileup effect (Cammin et al. 2014). When the pulse pileup effect is severe, the peak and valley of the

measured attenuation curve may also disappear. In this extreme case, the proposed energy calibration method fails. In the results presented in this paper, x-ray exposure levels have been selected to avoid the presence of strong pulse pileup effect. Second, the accurate statistical distribution of the K-edge threshold value $\hat{T}_k$ is not known. The assumed uniform distribution statistical model in this new method may introduce potential bias to the measured PCD threshold value $\hat{T}_k$ that corresponds to the material K-edge energy E_k .

Without knowing more prior information, this assumption of uniform distribution statistics is the most conservative one that can be made. In future work, other statistical models may be investigated to seek an improvement in the accuracy of determining the measured PCD threshold that corresponds to the material K-edge energy. Third, to illustrate the proposed method, a Gaussian blurring kernel was used (see Eq. (2)). However, the proposed energy calibration method does not depend on this assumption. The proposed calibration method only relies on the identification of a peak and a valley in the measured attenuation curve. As long as the peak and valley thresholds were identified, the uniform distribution assumption in the second discussion point was used to determine the threshold value for the K-edge. Finally, albeit the Gaussian kernel assumption was not the foundation of the proposed energy calibration method, this assumption is well valid around the main peak of the energy response curve as shown in our experimental results in figure 4 despite the existence of low energy continuum tail.

5. Conclusions

In conclusion, a new energy calibration method based on the measurements of material x-ray K-edge information has been developed for PCD energy calibration. Using this new approach, the linear relationship between the detector threshold and the x-ray photon energy can be obtained. The radioactive Am-241 isotope validation experiments have demonstrated good accuracy of this method.

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Figure 1.
The theoretical mass attenuation curves with K-edge for iodine, and the obtained energy dependent K-edge attenuation curves generated from three different PCD energy response functions.

Figure 2.

Experimental results of the measured energy dependent attenuation curves for three K-edge materials. From left to right, the three columns are for iodine, gadolinium, and gold, respectively. Results in the top row (a-c) are for the Hydra detector, and results in the bottom row (d-f) are for the Flite detector. The error bars represent the standard errors of the average attenuation over an ROI containing 2500 pixels.

Figure 3.

The energy calibration results for (a) Hydra, and (b) Flite detectors. The squares with error bars are the experimental data points, and the solid line is the linear regression result. The paired dashed lines define the 95% prediction intervals. The equation in each plot represents the linear relationship between the detector threshold T and the photon energy E .

Figure 4.

The measured spectrum of the radioactive isotope Am-241 from (a) Hydra, and (b) Flite detectors. Gaussian fittings were performed to obtain the central peak positions.

Table 1.

Detector threshold settings

K-edge material		Iodine	Gadolinium	Gold
Hydra	Min	31.0	61.0	101.0
	Max	69.0	109.0	183.0
	Window width T	2.0	2.0	2.0
Flite	Min	4.1	8.1	16.1
	Max	10.1	16.5	24.1
	Window width T	0.2	0.2	0.2

Table 2.

X-ray beam properties and exposure parameters

K-edge material	Iodine	Gadolinium	Gold
Tube potential (kV)	50	80	110
Added filtration	2 mm Al	2 mm Al	0.5 mm Cu
Tube current (mA)	15	12	3.3
Frame rate (Hz)	10	20	5
Number of frames for each energy window	50	50	50
Total mAs for each energy window	75	30	33

Table 3.

Results of the measured valley and peak threshold values, and the estimated PCD threshold values $\hat{T}_k$ at the K-edge energy

K-edge material		Iodine	Gadolinium	Gold
K-edge energy (keV)		33.2	50.2	80.7
Hydra	Valley	47.0	75.0	125.0
	Peak	63.0	97.0	161.0
	$\hat{T}_k \pm \sigma_{\hat{T}_k}$	55.0 ± 4.6	86.0 ± 6.4	143.0 ± 10.4
Flite	Valley	6.1	11.1	18.9
	Peak	8.3	14.5	23.1
	$\hat{T}_k \pm \sigma_{\hat{T}_k}$	7.2 ± 0.6	12.6 ± 1.0	21.0 ± 1.2