A Spectroscopic Monte-Carlo Model to Simulate the Response of Pixelated CdTe based Detectors

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Abstract

A fully spectroscopic Monte Carlo model has been developed to predict the spectroscopic performance of pixelated CdTe based detectors. The model incorporates photon attenuation by the photoelectric effect, Compton scattering and Rayleigh scattering. Charge transport equations are used to simulate the size of the electron cloud, approximated by a symmetrical two-dimensional Gaussian distribution, as it drifts to be read out at the detector anode. Direct comparisons are made between simulated data and an experimentally acquired spectra from a 1 mm thick CdTe sensor coupled to the HEXITEC detector ASIC. The probability of an absorbed photon leading to charge sharing across pixels as a function of incoming photon energy is investigated. The charge cloud size was found to be dominated by cloud growth during drift for photon energies < 100 keV. Furthermore, the portion of charge sharing events due to fluorescence from within the CdTe sensor is calculated – these events are distinguished from regular charge sharing events since their energy response differs. The model described is shown to give a good estimate of the total probability of charge sharing for energies up to 140 keV. CdTe sensor thickness, bias voltage, pixel size and electronic noise threshold can be adjusted to model a range of detector architectures.

Keywords: Monte Carlo detector model, CdTe, HEXITEC, Charge Sharing, Pixelated compound semiconductor detectors

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1. Introduction

Semiconductor radiation detectors based on compounds such as CdTe offer direct X-ray detection due to a high effective atomic number ($Z=50$) and density ($\sim 5.85 \text{ g/cm}^3$). Furthermore, CdTe's large bandgap results in low leakage current and noise [1], which in turn allows operation at room temperature with good spectral performance [2] without the need for cooling devices. For these reasons, CdTe sensor detector systems can be designed to achieve relatively conservative volume and power consumption, making them attractive candidates for hard X-ray and soft gamma-ray imaging and spectroscopy in nuclear medicine [3] and astronomy [4] applications.

Pixelating CdTe detectors has the obvious advantage of allowing imaging and, if the pixel pitch is small compared to the sensor thickness, mitigating the effects of poor hole mobility with the small pixel effect [5]. Material impurities and defects limit the charge carrier mobilities in these materials, particularly for holes, resulting in incomplete charge collection [1] and polarisation effects [6], thereby ultimately a reduction in spectroscopic performance. The small pixel geometry ensures that a significant charge is only induced by charge carriers drifting close to the anode pixel, described by the Shockley-Ramo theorem [7]. If the detector is back-illuminated such that the majority of interactions occur far from the anode, the detector will effectively become single carrier sensing in favour of the electrons by minimising the induced signal from the easily trapped holes, leading to better spectroscopic performance.

However, the downside to small pixel array detectors is that their performance suffers due to increased amounts of charge sharing [8]. Charge sharing occurs when the electron charge cloud from a single absorbed incident photon induces a charge across multiple pixels. The extent to which charge sharing occurs for these events, which will be referred to as shared events, depends on the initial charge cloud size, charge diffusion, Coulomb repulsion, X-ray fluorescence and Compton scattering. The process behind the formation of shared events is therefore quite complex, depending both on electron transport and secondary photon effects. Analytical models based on electron transport equations, which consider the geometrical and physical parameters of the detector and pixel array, have been used to estimate the amount of charge sharing across neighbouring pixels [8, 9, 10, 11]. In some cases these work well, but they do not factor in the influence of

the noise threshold or fluorescence photons on charge sharing, which have been shown to be significant [12]. In order to model stochastic effects such as X-ray fluorescence from the sensor material, Compton recoil electrons, photon pile-up and the distribution of electrons in a charge cloud, Monte-Carlo methods are needed. This has motivated the development of an end-to-end fully spectroscopic Monte-Carlo model, which can simulate the response of a pixelated CdTe detector for single pixel events and multipixel shared events.

In this work, the Monte Carlo model is described in detail and tested against experimental data obtained from observations using a 1 mm thick CdTe detector coupled to the HEXITEC ASIC [13]. The probability of an absorbed photon resulting in charge sharing is investigated as a function of the incoming photon's energy. Factors which influence the probability of charge sharing in pixelated CdTe detectors are discussed. Furthermore, charge sharing events that are due to photon fluorescence are distinguished from regular charge sharing events, and the relative incidence of each compared to experimental values.

2. Model

The Monte-Carlo model has been developed in the Python programming language [14] and can simulate the response of a pixelated CdTe detector for incoming photon energies ranging from 1 to 1000 keV. When the model is run, the interaction position of the incoming photon is determined by considering the photoelectric effect, Compton scattering and Rayleigh scattering. Secondary emissions such as X-ray fluorescence and Compton electrons are also considered. Once the interaction position is known, the electron transport of the charge cloud (approximated to be a two-dimensional Gaussian) as it drifts from its interaction position to be read-out at the anode is computed. The number of pixels the charge cloud spreads across, and how the charges are distributed amongst those pixels, is determined, as well as any charge loss due to charge trapping. The information containing the amount of charge collected in each pixel is stored in an event list, which is compiled from every photon (and its secondary emissions) introduced into the simulation. The event list can then be processed in the same manner as experimental data in order to reconstruct a spectrum for each event-type.

Figure 1 shows a schematic of how the detector is simulated within the model. The variables used in the schematic are referred to throughout this section.

Figure 1: Schematic of the CdTe detector as simulated by the model. The electrodes are positioned above and below the CdTe sensor in the middle. The entire CdTe sensor is assumed to be depleted by the electric field. The cathode is planar whereas the anode is pixelated. Although the cathode is drawn here, its attenuation is assumed negligible by the model. The thickness of the sensor is given by L and d is the drift length of the electrons to the anode. The electron charge cloud, as it is the one that is computed, is represented by a cone which increases in diameter as it moves towards the anode and spreads its charges over more than one pixel. The width of the Gaussian charge cloud (i.e. standard deviation) is given by σ .

2.1. Photon attenuation

The number of primary photons and their energy, E , is specified by the user. The photons are modelled as uniformly illuminating across the entire collecting area through the cathode and are assumed to be travelling perpendicular to the detector surface. Any attenuation by the cathode is taken to be negligible. The z -axis is defined to be from the cathode to the anode, measured from the surface of the sensor on the cathode side.

The attenuation depth, z , into the sensor from the cathode side for each photon is computed from the probability distribution obtained from the Beer-Lambert law [15]

$$P(z) = e^{-\mu(E)z} \quad (1)$$

where μ is the total linear attenuation coefficient of CdTe and depends on the energy E of the photon. The total linear attenuation coefficient is given by summing the sepa-

rate attenuation coefficients of the photoelectric effect, Compton scattering and Rayleigh scattering. Values for μ are taken from the National Institute of Standards and Technology (NIST) XCOM database [16], interpolated on a log-log scale. Photons for which z is greater than the thickness of the sensor pass through the sensor unattenuated and are consequently removed from the simulation.

2.1.1. Scattering

The relative attenuation cross-sections [16] at the photon energy E are used to determine the type of attenuation at position z . For the Photoelectric effect for example, the relative attenuation $P_{\mu_{pe}}$ is

$$P_{\mu_{pe}} = \frac{\mu_{pe}(E)}{\mu(E)} \quad (2)$$

where μ_{pe} is the attenuation coefficient for the photoelectric effect only. If attenuation occurs via the photoelectric effect, the primary photon is assumed to be completely absorbed at depth z . Otherwise, the photon is scattered by either Rayleigh or Compton scattering (determined by the relative attenuations). The scattered photons either interact at a new position, or escape the sensor and are removed from the simulation. This step is repeated until all scattered photons have either been absorbed in the sensor or escaped. The distance the scattered photons travel before interacting again is calculated using equation 1.

In the case of Rayleigh scattering, since it is a form of coherent scattering, the scattered photon does not transfer any of its energy to an electron. Instead, only the direction of travel of the photon changes. The possible scattering angles are defined by a probability distribution that depends on the energy E of the photon being scattered and the Z number of the atom involved in the interaction [17]. Since Z will depend on whether the photon interacts with a Cd or Te atom, the atom the photon interacts with is first determined. The probability, P , of the photon interacting with a Cd atom, for example, is [18]

$$P = W_{Cd} \frac{\left(\frac{\mu}{\rho}\right)_{Cd}}{\left(\frac{\mu}{\rho}\right)_{CdTe}} \quad (3)$$

99 where W_{Cd} is the weight fraction of Cd in CdTe (0.468) and ρ the density of the material
100 [16].

101 When Compton scattering occurs, the primary photon imparts some of its energy
102 to the electron it interacts with and is scattered in a new direction. The energy of the
103 scattered photon, E' , is defined by [19]

$$E' = \frac{E}{1 + \frac{E}{m_e c^2} (1 - \cos \theta)} \quad (4)$$

104 where θ is the scattering angle, m_e the electron mass and c the speed of light. Compton
105 scattered photons are assumed only to interact with free electrons. The Klein-Nishina
106 formula [20] is therefore used to determine θ from the probability distribution function
107 of all possible scattering angles for a photon with energy E . The energy absorbed by
108 the Compton scattered electron at the interaction position is then

$$E_e = E - E' \quad (5)$$

109 2.2. Absorption

110 At this stage, all primary and scattered photons have either been absorbed via the
111 photoelectric effect or escaped the sensor. The energy a primary or scattered photon
112 deposits at the interaction position is dependent on the atom and shell it is absorbed by,
113 and any resulting fluorescence photons.

114 The atom the photon interacts with is determined using equation 3. The shell the
115 photon interacts with will first depend on the binding energy of the shells relative to the
116 energy of the photon. If the energy of the photon does not exceed the binding energy E_b
117 of a shell, absorption by that shell is not possible. The binding energy of the shells are
118 taken from [21]. Where $E > E_b$, the shell the photon is absorbed by is determined by
119 comparison of the mass attenuation coefficients of the individual shells. Electrons bound
120 to the K, L₁, L₂ and L₃ shells are considered in the model. The mass attenuation for an
121 individual shell can be calculated from the total mass attenuation of the atom and its
122 jump factor, J , [18]

$$\left(\frac{\mu}{\rho}\right)_{shell} = \frac{J-1}{J} \left(\frac{\mu}{\rho}\right)_{tot} \quad (6)$$

123 The jump factor is the fraction of the total photoelectric absorption coefficient due
 124 to absorption by electrons of the respective shell.

125 2.2.1. Fluorescence

126 A vacancy is created in the shell that the photon interacts with. The fluorescence yield
 127 for the respective shell is used to determine if the filling of the vacancy by a cascading
 128 electron results in a fluorescence photon. If fluorescence does not occur, the complete
 129 energy of the primary photon is assumed to be absorbed by the photoelectron such that
 130 $E_e = E$. If a fluorescence photon is emitted from the atom, the relative radiative rates
 131 are used to determine which transition has occurred. Possible transitions, their line
 132 energies and their relative rates for both Cd and Te are shown in table 1 [21]. A vacancy
 133 that forms in an L-shell of the same atom due to a $K\alpha$ transition, may also fluoresce and
 134 that fluorescence photon may then escape the atom too. The energy of the photoelectron
 135 E_e , where fluorescence does occur, is therefore

$$E_e = E - \sum_{i=1}^n E_{fl_i} \quad (7)$$

136 where E_{fl_i} is the energy of the fluorescence photon from the i th shell. Vacancies that
 137 arise in an M or N shell due to the cascading of electrons or otherwise, are ignored. Given
 138 that the binding energy for these shells is very small (e.g. 0.618 keV for M_3 shell in Cd
 139 [21]), and that any resulting fluorescence will consequently be of very low energy (0.603
 140 keV for M_γ line [22]) and is therefore most likely to be reabsorbed close to the original
 141 vacancy (mean path length of 1 keV in CdTe is $0.2\mu m$), the energy from these shells
 142 is assumed not to escape the pixel and is instead included in the primary photoelectron
 143 energy.

144 The direction of the fluorescence photons is uniformly distributed over all solid an-
 145 gles. The steps described so far for the primary photons are repeated for the secondary
 146 fluorescence photons and any further fluorescence photons that result from those. When
 147 absorption by K and L shells can no longer occur (i.e. when the energy of all remaining
 148 photons is less than the binding energy of the Cd L_3 shell, 3.537 keV [21]), the remaining
 149 photons are assumed to be absorbed in either an M or N shell (if they have not escaped
 150 the sensor).

Transition	Cd		Te	
	Line energy (keV)	Rate	Line energy (keV)	Rate
$K\alpha_1$ (KL ₃)	23.174	0.55	27.473	0.53
$K\alpha_2$ (KL ₂)	22.984	0.29	27.202	0.29
$K\beta_1$ (KM ₃)	26.095	0.09	30.996	0.10
$K\beta_2$ (KM ₂)	26.654	0.02	31.700	0.03
$K\beta_3$ (KM ₂)	26.061	0.05	30.945	0.05
$L\alpha_1$ (L ₃ M ₅)	3.134	0.77	3.769	0.75
$L\alpha_2$ (L ₃ M ₄)	3.127	0.08	3.758	0.08
$L\beta_2$ (L ₃ N ₄)	3.528	0.12	4.302	0.14
Ll (L ₃ M ₁)	2.767	0.03	3.336	0.03
$L\beta_1$ (L ₂ M ₄)	3.317	0.91	4.030	0.88
$L\gamma_1$ (L ₂ N ₄)	3.717	0.09	4.571	0.12
$L\beta_3$ (L ₁ M ₃)	3.401	1.00	4.120	1.00

Table 1: Possible transitions for Cd and Te atoms used in the model, along with line energies and relative radiative rates for each transition [21] rounded to three and two significant figures.

2.3. Charge transport

At this stage, the initial position of each photoelectron from absorbed primary and secondary photons is known. The photoelectron will lose energy by ionisation, creating electron-hole pairs along its path until it is stopped. The number of electron-hole pairs, N , is given by

$$N = \frac{E_e}{\omega} \quad (8)$$

where ω is the average pair creation energy, equal to 4.3 eV in CdTe [1]. The variance on N is described by the Fano-noise and is assumed to follow Fano adjusted Poisson statistics ($\sigma_N^2 = FN$). The Fano factor, F , is taken to be 0.1 for CdTe [23].

159 2.3.1. Charge cloud size

160 The charge cloud is modelled as a symmetrical two dimensional Gaussian distribution
 161 [24, 25] perpendicular to the direction of the electric field lines (i.e. the z-axis). The
 162 final size of the cloud will depend on the initial size, σ_i , from the excitation of electron-
 163 hole pairs by the photoelectron and the growth of the cloud, σ_d , due to diffusion and
 164 electrostatic repulsion of the charges as the cloud drifts to the anode. The size of the
 165 charge cloud σ at the anode is described by adding the two components in quadrature
 166 within the assumption that their magnitudes are independent of one another

$$\sigma = \sqrt{\sigma_d^2 + \sigma_i^2} \quad (9)$$

167 The cloud growth due to diffusion, σ_d , can be calculated using the diffusion equation
 168 derived from Fick's second law [26]

$$\frac{\partial \sigma_d(t)^2}{\partial t} = 2D \quad (10)$$

169 where D is the diffusion coefficient and $\sigma_d(t)^2$ is a function of time. The diffusion
 170 coefficient is given by the Einstein relation [27]

$$D = \mu_e \frac{k_b T}{q} \quad (11)$$

171 where μ_e is the electron mobility, k_b Boltzmann's constant, q the elementary charge
 172 and T the temperature of the sensor. The total drift time t_d for the electron cloud to
 173 reach the anode is equal to

$$t_d = d \frac{L}{\mu_e V} \quad (12)$$

174 where L is the thickness of the CdTe sensor, d the drift length of the electron cloud
 175 to the anode (given by $L - z$) and V the applied bias voltage. The electrostatic repulsion
 176 during drift is included by using an effective diffusion constant D' [24] in place of D in
 177 equation 10

$$D' = D + \frac{\mu_e N q}{24\pi^{3/2}\epsilon} \frac{1}{\sigma(t)} \quad (13)$$

where ϵ is the permittivity in CdTe and $\sigma(t)$ is the size of the electron cloud after some arbitrary amount of time t . By combining equations 10, 11 and 13, the differential equation which gives the size of the electron cloud due to diffusion and repulsion is

$$\frac{\partial \sigma_d(t)^2}{\partial t} = \frac{2\mu_e k_b T}{q} + \frac{\mu_e N q}{12\pi^{3/2}\epsilon} \frac{1}{\sigma(t)} \quad (14)$$

A numerical solution is found for σ_d by using the 4th order Runge-Kutta method over 10^3 time steps between $t = 0$ and $t = t_d$. At $t = 0$, the size of the electron cloud $\sigma(t)$ is assumed to be equal to σ_i . Once equation 14 has been solved, equation 9 is used to compute the final size of the electron cloud.

GEANT simulations by Blevis and Levinson [28] give estimates for the initial charge cloud size generated by a photoelectron at different energies, which have previously been used in Monte-Carlo simulations to model X-ray spectra from a CdTe detector [25]. The values used for σ_i in this work are 0 μm , 1 μm , 4 μm at electron energies of 0 keV, 35 keV and 100 keV. A second order polynomial fit is used to extract σ_i for each absorbed photoelectron energy E_e in the simulation.

2.3.2. Charge collection efficiency

As charges drift to an electrode, they can become trapped in defects and impurities in the crystal resulting in charge loss and therefore incomplete charge collection. To account for this effect, the Hecht relation [29], which calculates the charge collection efficiency (*CCE*), is used

$$CCE = \frac{\lambda_h}{L} \left(1 - e^{-\frac{\psi(z)}{\lambda_h}} \right) + \frac{\lambda_e}{L} \left(1 - e^{-\frac{\psi(L-z)}{\lambda_e}} \right) \quad (15)$$

where $\lambda_h = \mu_h \tau_h E_f$, $\lambda_e = \mu_e \tau_e E_f$ are the mean drift lengths of holes and electrons respectively, and are a product of the carrier lifetime τ , the carrier mobility μ and the electric field strength E_f . The electric field is assumed to be uniform across the sensor (i.e. an effective electric field strength is used to account for a non-uniform field, see section 4.1). The weighting potential, ψ , takes into consideration the geometry of the sensor and correctly describes the relative current that the respective charge carrier can induce on the anode. Figure 2 shows the weighting potential for the HEXITEC CdTe detector for which $w/L = 0.25$, where w is the size of the pixel pitch [30]. The curve for

204 a planar detector where the pixel size is equal to or greater than the sensor thickness
 205 is shown for comparison. The weighting potential therefore describes the effect of the
 small pixel geometry.

Figure 2: Weighting potential for a planar detector ($w/L \geq 1$) and for the geometry of the HEXITEC CdTe sensor. The left-hand y-axis is the weighting for the holes and therefore the cathode side. The right-hand y-axis is the weighting for the electrons and therefore the anode side.

206
 207 The *CCE* is calculated for each electron charge cloud by first sampling the weighting
 208 potential at the interaction depth z and then using equation 15. The effective number
 209 of charges that is equivalent to the current that is actually induced on the anode, N' , is
 210 then

$$N' = CCE \times N \quad (16)$$

211 2.3.3. Pixel readout

212 For each charge cloud, a two-dimensional Gaussian distribution with standard de-
 213 viation σ , containing N' charges, is evaluated against the pixelated array, centred on
 214 the absorption position. The charges in each pixel are summed to obtain the energy
 215 deposited in that pixel. The model does not simulate charge loss across the inter-pixel
 216 region.

Electronic noise is added to each pixel that contains an energy. The electronic noise is assumed to follow a Gaussian distribution with variance $\sigma^2 = A$ where A is equal to the equivalent noise charge (ENC). The ENC is a free parameter in the model that can be adjusted to match experimental data.

An eventlist containing the charge collected in each pixel for every frame in the simulation is saved. Secondary emissions are assumed to happen instantaneously and are therefore recorded in the same frame as the primary photon which triggered them.

2.4. Spectral response reconstruction

The structure of the eventlist generated by the model is identical to the format in which the experimental data from the HEXITEC ASIC is recorded. Simulated event lists are therefore processed using the analysis algorithm for experimental data described by Bugby et al [12].

The algorithm classifies the type of each event. Pixels that are adjacent to one another are said to be part of the same event. The event type then depends on the number of pixels the event contains – the considered event types are shown in figure 3. The energy of an event is the sum of the energy in all pixels of that event. A separate spectrum is reconstructed for each event type, where only events with a shape as it is shown in figure 3 are included, such that linear tripixels and quadpixels for example (which were more likely to exhibit photon pileup) are not added to their event type spectrum. Different orientations for identically shaped events showed no difference in their energy response and are therefore considered as the same event type. Diagonally adjoined events are counted as two separate events [12].

It is common practise to apply a noise threshold to the energy in each pixel of an observation in order to remove counts that are due to thermal charge leakage from the crystal and detector electronics, instead of an absorbed photon. The noise threshold is applied by the algorithm – removing all pixels in an event that have an energy lower than the threshold.

3. Detector description

The detector system used in this work is the STFC High Energy X-ray Imaging Technology (HEXITEC) [13], developed to detect hard X-rays and gamma rays. The

Event type	Event shape	Event type	Event shape
1: Isolated		3: Tripixel
2: Bipixel		4: Quadpixel

Figure 3: Events shapes for isolated, bi-, tri- and quad- pixel events. The greyed shaded squares correspond to pixels which have recorded an energy greater than the noise threshold.

HEXITEC consists of a detector that is coupled to an ASIC to perform spectroscopic observations. The ASIC is pixelated by an 80 x 80 array with a pitch of 250 μm manufactured on a standard 0.35 μm CMOS (complementary metal-oxide semiconductor) process, such that each ASIC pixel contains a charge amplifier, shaping amplifier and a peak track-and-hold circuit. Therefore, induced charge is converted to a voltage at the pixel level, allowing each pixel to provide a full energy spectrum. The design of the detector consists of a platinum planar cathode and pixelated aluminium anode on opposite sides of a CdTe semiconductor material. The CdTe sensor has a thickness of 1 mm and a 20 x 20 mm collecting area. The anode is pixelated by an 80 x 80 array with a pixel electrode size of 200 μm and an inter-pixel spacing of 50 μm . The ASIC and anode are attached by flip-chip assembly to gold studs placed on each of the ASIC bond pads.

The HEXITEC system has shown good spectral result room temperature with a CdTe sensor [31], achieving a mean FWHM energy resolution for all pixels of 0.75 keV for incoming photons of energy 59.5 keV.

4. Data collection

4.1. Simulated data

For each simulation, the model was run with 10^7 primary photons and with a sensor temperature of 28°C.

Cola et al. show that when applying a bias voltage of -500 V, the effective voltage is in fact -425 V because of a nonuniform electric field across the sensor thickness which decreases with distance from the anode [32]. Test simulations were performed using the nonuniform electric field profile shown in [32] when applying a -500 V bias. However, comparative simulations using an equivalent effective bias voltage and a uniform field produced the same results. Therefore, in the interest of reducing computation time, the effective value is used for the bias voltage in the simulations.

Since the model does not distinguish between the inter-pixel gap and the pixel electrode, the pixel size used in the simulations is the electrode size of 200 μm on a 80 x 80 pixel array. Charge induction maps show that electric field lines at the anode still detect electrons from the inter-pixel region, with the field lines from the gap's neighbouring pixels sharing the inter-pixel region equally [33].

The ENC was set to 60 electrons rms in order to match the FWHM of the simulated photopeaks to that of the experimental photopeaks for isolated events. An energy bin size of 0.3 keV and a noise threshold of 3 keV were used.

4.2. Experimental data

The energy response in each pixel of the detector was calibrated using the methods previously reported in [12]. Table 2 lists the sources and line energies used for calibration.

As K-shell X-ray fluorescence is known to have an effect on charge sharing in CdTe [8], peaks closer to the absorption edges of CdTe ($\sim 26\text{-}31$ keV) were desirable. An X-ray tube (Amptek Mini-X [35]), was used to obtain additional photopeaks could be obtained at 32.5 keV, 38.0 keV and 45.8 keV. The tip of the Amptek X-ray tube was placed 3 cm from the surface of the detector and equipped with a 2 mm collimator. A silver (Ag) transmission target was used to obtain the three photopeaks, with electrons accelerated at the target across a tube voltage of 35 kV, 40 kV and 50 kV. Since only photons above the CdTe absorption edges were of interest, Niobium (Nb), Gold (Au) and Chromium (Cr) filters were used to remove lower energy photons. Therefore, peaks were effectively created from the bremsstrahlung continuum emitted from the X-ray tube. Table 3 shows the additional peaks acquired from the X-ray tube measurements and the filter(s) used, and table 4 gives details on the filters.

Source	Source activity (MBq)	Photopeak energies (keV)	Acquisition time (s)	Frame occupancy (%)
^{109}Cd	84.9	22.00 ± 0.10	1000	0.4
		24.90 ± 0.01		
		88.00 ± 0.01		
^{241}Am	351.7	59.54 ± 0.01	1000	0.5
^{57}Co	51.7	14.40 ± 0.10	7000	0.2
		122.10 ± 0.05		
		136.50 ± 0.10		
^{55}Fe	414	5.95 ± 0.01	3600	0.2
$^{99\text{m}}\text{Tc}$	188.3	140.50 ± 0.01	1800	0.4

Table 2: Photopeak energies obtained from experimental flood images taken by [12] using different radioisotope sources. Multiple peaks (i.e. $K_{\alpha 1}$ and $K_{\alpha 2}$) have been combined into a single peak energy taking into account their relative intensity where these cannot be resolved. The range of energies included in each photopeak is shown as a standard error, this is set to a nominal value of 10 eV when individual peaks have not been combined. The frame occupancy is the mean percentage of pixels in each frame which are above the noise threshold [34].

Figure 4 shows the event type spectra for the 40 kV and 50 kV tube voltage acquisitions. It can be seen that the bremsstrahlung peaks for all event types are well separated from the lower energy peaks coming from the Ag X-ray tube target and Nb filter K-shell fluorescence in the case of the 50 kV observation. This meant that charge sharing at the energy of the main photopeak could be analysed without any interference, identically to the radioisotope source peaks. However, since the X-ray tube acquired photopeaks are not from a discrete energy as for the radioisotope peaks, and have a FWHM of ~ 7 keV, the uncertainty on the energy for the peaks acquired from these observations is ± 3.5 keV.

For all acquisitions, the detector was run with a bias voltage of -500 V and the detector temperature was observed to remain at $28 \pm 1^\circ\text{C}$. The bias voltage was periodically refreshed by switching the bias to 0 V for 2 seconds every 60 seconds. This was done

Tube voltage (kV)	Tube current (μ A)	Photopeak energy (keV)	Acquisition time (s)	Frame occupancy (%)	Filter(s) used		
					Au	Cr	Nb
35	110	32.5 ± 3.5	1800	0.2	X		
40	80	38.0 ± 3.5	1800	0.2	X	X	
50	5	45.8 ± 3.5	1200	0.2			X

Table 3: Photopeak energies obtained from X-ray tube measurements by accelerating the electrons with different electric field strengths. The uncertainty of the photopeak energies is determined from the peak FWHM. The applied filter(s) is marked by an X.

Filter	Density (g/cm ³)	thickness (mm)	Fluorescence X-ray emission (keV)	
			K $_{\alpha}$	K $_{\beta}$
Au	19.32	0.25	68.12 ± 0.10	77.98 ± 0.01
Cr	7.19	1.00	5.41 ± 0.05	5.95 ± 0.01
Nb	8.57	1.00	16.50 ± 0.10	18.62 ± 0.01

Table 4: The different filters used for the X-ray tube measurements shown in table 3. The K-shell fluorescence photon emission energies from the filters is also shown. The K $_{\alpha 1}$ and K $_{\alpha 2}$ peaks were combined and errors were determined in the same way as for the photopeaks in table 2.

to prevent known time-dependent polarisation effects of Schottky contact CdTe [6]. To minimise the likelihood of shared events occurring due to photon pileup, it was ensured that the frame occupancy in each observation did not exceed 1%.

The spectral reconstruction algorithm described in Section 2.4 was used on the raw experimental data files to build the energy spectra. An energy bin size of 0.3 keV and a noise threshold of 3 keV were used.

5. Comparison with measurement

5.1. Simulated spectral detector response

The Monte-Carlo model was tested against experimental data by simulating the detectors response to an ²⁴¹Am source and comparing to the experimental spectrum, shown in figure 5. The model can only accurately simulate the peak width for isolated events

Figure 4: The spectrum for isolated, bipixel, tripixel and quadpixel events detected with the HEXITEC from the 40 kV (Top) electron accelerated X-ray tube acquisition using the Au and Cr filters, and 50 kV (Bottom) electron accelerated X-ray tube acquisition using the Nb filter. The photopeaks for the multipixel events are positioned at a lower energy due to charge loss to the inter-pixel gap.

as it does not account for the charge loss across the inter pixel gap for shared events. Therefore, only the spectrum from isolated events is compared. The simulated and experimental data are normalised by the maximum number of counts in an energy bin of the primary photopeak.

The detector response to the ^{241}Am source is dominated by the primary gamma emission line at 59.5 keV. The lower energy X-ray L-shell lines from the ^{241}Am decay product ^{237}Np are not observed due to shielding from the 0.5 mm thick steel source housing. Attenuation by the source housing was also applied to the simulated data. All the peaks seen in figure 5 and their measured positions from experiment and simulation are listed in table 5. The escape peaks are due to fluorescence escaping a pixel which absorbed a 59.5 keV photon, by either leaving the sensor or being reabsorbed beyond the nearest pixel neighbours. The escaped fluorescence photons which are reabsorbed within the sensor lead to the fluorescence peaks at ~ 23 and ~ 26 keV. The total number of 59.5 keV absorbed isolated events is the sum of all counts in the primary gamma photopeak

Figure 5: Experimentally observed ^{241}Am spectrum compared with the simulated response to the same source. The spectra are normalised to the maximum counts in an energy bin of the 59.5 keV photopeak and only include isolated events. The shaded regions highlight the energy windows used to calculate the total number of counts belonging to each peak.

and all escape peaks. The proportion of counts in each of the other peaks are shown in table 5, with good agreement between experimental and simulated values. The energy windows used around each peak for calculating the proportions are shown in figure 5 by the shaded regions underneath the simulated curve and also written in table 5.

The simulated response reproduces the low energy tail seen in the experimental spectrum on the LHS of the 59.5 keV photopeak. The tail arises due to two distinct mechanisms. The first is due to the noise threshold, which removes any energy belonging to the main event that is in an adjacent pixel and lower than the noise threshold. The second is a consequence of the hole trapping which results in hole tailing [23] as charge from trapped holes is not fully collected. Both mechanisms are considered in the model, with the latter process taken into account by the charge collection efficiency (*CCE*) used with the appropriate weighting potential for the small pixel geometry of the detector (Section 2.3.2).

Peak	Peak position (keV)		Energy Window (keV)	Proportion of counts (%)	
	Experiment	Model		Experiment	Model
γ	59.5	59.5	50 - 62	85.0 ± 1.0	84.0 ± 0.8
Cd K_{α} escape	36.2	36.4	35 - 38	6.6 ± 0.3	7.9 ± 0.2
Cd K_{β} escape	33.1	33.4	31 - 34.5	6.7 ± 0.3	6.7 ± 0.3
Te K_{α} escape	31.9	32.1			
Te K_{β} escape	28.4	28.5	27.5 - 29.5	1.8 ± 0.4	1.4 ± 0.3
Cd K_{β}	26.0	26.0	25 - 27	3.1 ± 0.4	1.9 ± 0.2
Cd K_{α}	23.0	23.0	22 - 24	3.6 ± 0.2	4.2 ± 0.1

Table 5: All visible peaks in the ^{241}Am spectrum and their peak energy positions as measured from the experimental and simulated data shown in figure 5. The energy window corresponds to the shaded region underneath the respective peak in figure 5. The percentages are the proportion of counts in the respective peak from the total number of absorbed incident isolated events (i.e. γ photopeak and escape peak counts summed). The errors for the proportion of counts were determined by increasing the energy window by 0.5 keV at both the lower and upper bound and calculating the difference.

5.2. Shared events

The probability of a shared event occurring due to charge sharing was investigated as a function of energy from the experimentally acquired data and compared with simulations. The detector response was simulated at multiple energies covering the experimental photopeak energy range from 5.95 keV to 140.5 keV. For both experiment and simulation, the event list for each observation was analysed using the reconstruction algorithm described in Section 2.4 – producing a spectrum for each event type of interest. An energy noise threshold of 3 keV was applied.

5.2.1. Energy response of shared events

Figure 6 shows the different event type spectra for the ^{109}Cd and ^{57}Co experimentally acquired data. Photopeaks made of multi-pixel event types are much broader than the equivalent isolated event type photopeak. This is due to the effect of charge loss, partially caused by charges drifting in the inter-pixel region [33]. The reasons behind charge loss

Figure 6: Event type spectra for ^{109}Cd (LHS) and ^{57}Co (RHS) from experimental observations.

across the pixel gaps are described in more detail in [12]. However, some charge sharing events do not exhibit as much, if any, charge loss. This can be seen by the 122 keV photopeak (^{57}Co source) in the bipixel event spectrum which shows two components – a peak at 121 keV followed by a flat shoulder at lower energies. This is believed to be due to two types of shared events – those created by fluorescence and those solely created by the charges from one cloud centre spreading. In the case of fluorescence shared events, a fluorescence photon escapes into a pixel adjacent to the pixel of the incident photon and deposits its energy there directly. The shared event is not created by charges spreading across the inter-pixel region, as is the case for the other type of shared event, and therefore does not suffer from charge loss. For the 22 keV photons in the ^{109}Cd bipixel spectrum, no two distinct peak components can be seen. Since K-shell fluorescence does not occur at this energy, all of the counts in the ^{109}Cd bipixel photopeak suffer from charge loss, shifting the peak to 19.5 keV.

Figure 7 shows the energy split across the two pixels for all 59.5 keV ^{241}Am bipixel events. The straight line indicates the case in which no charge loss occurs – along which summing the energy in the two pixels always equals the known photopeak energy of 59.5 keV. The actual distribution deviates from this line due to the charge loss in the charge spreading shared events. The bright spots in figure 7 correspond to the fluorescence

376 shared events. The fluorescence spots are along the straight line, indicating these events
 377 do not suffer from charge loss.

Figure 7: Two-dimensional histogram showing the distribution of split energies for all bipixels in the energy range from 50-62 keV for the ^{241}Am data. The straight yellow line shows the ideal case in which no charge loss occurs. The gaps on either axis from 0-3 keV correspond to the noise threshold. The bright spots are annotated with the fluorescence photon which causes the bipixel event. In total there are eight bright spots - only four are annotated because the remaining four are the same but with the energies in opposite pixels.

378 5.2.2. Probability of a shared event

379 For both the experimental and simulated data, the likelihood of the event types
 380 introduced in figure 3 occurring at a given energy was determined. This was done by
 381 using energy windows around the photopeaks of interest and counting the number of
 382 events belonging to each specific event type. The number of counts of each event type
 383 was normalised by the total number of counts including all event types for the given
 384 photopeak.

385 Figure 8 shows the experimentally calculated probability of any shared event occur-
 386 ring at the incoming photon energies listed in table 6, compared with the simulated result
 387 at the same energies and some additional energies. The individual probabilities of the

Source	Peak energy (keV)	Energy window (keV)			
		Isolated	Bipixel	Tripixel	Quadpixel
^{55}Fe	5.95 ± 0.01	4-11	4-11	4-11	4-11
^{109}Cd	23.10 ± 1.00	13-28	12-28	13-28	14-28
	88.00 ± 0.01	77-92	75-91	73-91	73-91
^{241}Am	59.54 ± 0.01	39-63	38-63	37-63	37-64
^{57}Co	14.40 ± 0.10	9-16	6-16	6-15	11-16
	74.00 ± 1.00	63-77	60-76	59-75	59-73.5
	122.10 ± 0.05	105-126	105-126	105-125	105-124
	136.50 ± 0.10	126-140	125-140	124-140	123-140
^{99m}Tc	140.50 ± 0.01	125-145	120-145	120-145	118-145
X-ray tube (35 kV)	32.5 ± 3.5	27-36	25-36	23-36	23-36
X-ray tube (40 kV)	38.0 ± 3.5	28-42	28-42	28-42	28-42
X-ray tube (50 kV)	45.8 ± 3.5	31-51	26-50	24-49	25-48

Table 6: Photopeak energies at which the probability of charge sharing is calculated. The data and analysis for the peak energies obtained from the radioisotope sources is from [12]. The peaks observed from the X-ray tube experiments are from this work. The 74 keV energy analysed from the ^{57}Co acquisition data occurs due to Pb fluorescence from shielding in the experimental setup. The peak energy uncertainties have been defined in the same manner as in table 2. The ^{109}Cd 22.00 keV and 24.90 keV peaks have been combined and are treated as a single photopeak with average energy of 23.10 keV when considering the relative intensities. The energy windows used for each event type for the experimental spectra are also given.

different event types occurring as a function of incoming photon energy, are shown in figure 9 for both the experimentally calculated result and the model prediction. Errors for the event type probabilities are estimated at $\leq 2\%$ due to Poisson counting statistics and the dependency on the position of the energy window.

Both the experimental result and model prediction shown in figure 8 suggest that the probability of a shared event occurring increases rapidly at lower energies until reaching 50% at ~ 50 keV. The shared events probability then increases gradually to 62.5% at

Figure 8: The probability of any type of shared event to occur as a function of incoming photon energy, calculated from experiment and as predicted by the model. The data points mark the energies at which the calculations/simulations were performed. A low noise energy threshold of 3 keV was applied.

140.5 keV.

The trend of the probability of charge sharing with energy is estimated well by the model. The steep increase in shared events at lower energies is due to the noise threshold. At these energies, energy shared with adjacent pixels is more likely to be lower than the threshold, leading to a failure to identify true shared events. The sudden increase at ~ 26 keV (the K-edge of Cd) is due to the addition of fluorescence photons. These have mean attenuation ranges of around $100\mu\text{m}$ and can therefore escape into neighbouring pixels and create shared events. Alternatively, the fluorescence photons may escape beyond the neighbouring pixels, giving rise to the escape peaks. This has the effect of reducing the total number of isolated counts in the main photopeak and therefore also increasing the percentage of shared events at that energy. For the Te K-edge at ~ 32 keV there is another sudden jump in the shared events probability, although this is much smaller due to the shorter range ($\sim 60\mu\text{m}$ mean attenuation length) of the Te K-shell fluorescence photons in CdTe. However, the Te K-shell fluorescence photons have energies (27 keV -

Figure 9: Probability of the individual event type to occur as a function of incoming photon energy. The solid lines are the model prediction, and the dashed lines, with the data points, the experimental result. An low noise energy threshold of 3 keV was applied.

31 keV) above the binding energy of the K-shell in Cd. Therefore, if reabsorbed, they can cause additional K-shell fluorescence from the Cd atoms, resulting in pushing the shared events probability up further. Directly after the absorption edges, the shared event probability continues to increase at a relatively steep rate before levelling off. Levelling off is expected to occur at ~ 35 keV, which is where the energy that remains in the pixel after the fluorescence photon escapes, is still above the 3 keV noise threshold. From ~ 40 keV upwards, there is then a gradual increase in the probability of a shared event as the final cloud size becomes increasingly dependent on the width of the initial excitation of charge carries from the photoelectron, rather than on the cloud growth during drift.

figure 9 shows that the majority of the shared events within the investigated energy range are bipixels. Although the total charge sharing probability between the simulated and experimental data agrees very well, the relative contribution of the event types differ at higher energies. The simulated data predicts more bipixels and fewer quadpixels than what is observed experimentally. Furthermore, the simulated results do not show a jump in the probability for quadpixels after the Cd K-edge as suggested by experiment.

Figure 10: The average charge cloud size at different energies due to the initial width and due to growth during drift to anode as predicted by the model. The combined average total size is also shown. The model was simulated between 1 and 141 keV with 1 keV intervals - only the curve is shown.

Figure 10 shows the average contribution to the final cloud size at the anode in terms of the σ of the two distinct components (drift and initial size), as predicted by the model. This suggests that the final cloud size is dominated by the growth due to diffusion and electron repulsion during drift towards the anode up to ~ 100 keV. The average total charge cloud size is found to be relatively constant between 1 and 100 keV at $\sigma \approx 13 \mu\text{m}$. A charge cloud containing $\sim 99.7\%$ (i.e. $\pm 3\sigma$) of all charges therefore extends $\sim 78 \mu\text{m}$ in diameter. Above the Cd and Te K-edges, photons are again absorbed closer to the cathode, increasing the drift time of the excited charges and therewith the cloud size. The relatively constant cloud size supports the argument that at low energies it is the noise threshold that prevents much larger portions of shared events.

5.2.3. Portion of fluorescence shared events

In Section 5.2.2 it was shown that fluorescence from the CdTe crystal itself has a considerable impact on the probability of charge sharing. Fluorescence shared events suffer less from charge loss and as a result show better energy resolution and can be

recombined through simple addition to recover the original photon energy. [12]. It is therefore of interest to quantify the portion of shared events that are due to fluorescence.

Using the data in figure 7 from section 5.2.1, the portion of bipixels at 59.5 keV that are only due to fluorescence were calculated. This was done using two-dimensional energy windows around the bright fluorescence spots in the image, summing the number of counts in those regions and normalising by the total number of bipixels. The same plot and analysis was performed using simulated data at 59.5 keV. Furthermore, both experimental and simulated calculations for the portion of fluorescence shared events were repeated for the 122 keV line. Table 7 shows the results from these calculations.

Figure 11: Each image is a distribution of the energy in the two non-maximum pixels from ^{241}Am 59.5 keV tripixel events. The two rows of images correspond to experiment and simulation respectively. Each column of images corresponds to one of the specific tripixel event types - centre, edge, outer line and centre line events. A drawing of the pixels making up the tripixel event type is shown in the first image of each column, with the filled pixel indicating the pixel containing the maximum energy.

The analysis carried out on the bipixels was extended to tripixel events. In order to determine the portion of tripixels due to fluorescence, the tripixels themselves were

449 further separated into four types. These types are centre events, where the pixels make a
 450 right-angle and the maximum energy is recorded in the centre/middle pixel, edge events,
 451 where the pixels also make a right-angle but the maximum energy is recorded in one of
 452 the outer end pixels and two types of line events where the three pixels are orientated
 453 in a line and the maximum energy is either in an outer or centre pixel. The four tripixel
 454 event types are shown in figure 11 – the filled pixel signifies the pixel with the maximum
 455 recorded energy.

456 The majority of tripixel events were found to be in the right-angle arrangement for
 457 both the 59.5 keV and 122 keV line energy, at 93.0% and 91.5% respectively, with the
 458 rest being line events.

459 The location of the maximum energy pixel in a tripixel event, is an indication of
 460 whether charge sharing occurred due to fluorescence or charge spreading. This can be
 461 seen in figure 11 which shows the distribution of the energy in the remaining two non-
 462 maximum pixels for each of the four tripixel types. By visual inspection, it is clear the
 463 distributions for the edge events and centre events are distinctly different. Edge events
 464 are mostly made up of events where summing the energy in the two non-maximum pixels
 465 equals the energy of Cd (~ 23 keV) or Te (~ 26 keV) K-shell fluorescence. For example
 466 at the bright streaks in the distribution at 20 and 23 keV. Counts along the downwards
 467 sloping curve are cases where the energy from the fluorescence photon spreads between
 468 the two non-maximum pixels. This leads to charge loss across the pixel gap, giving rise
 469 to the non-linear curve as observed previously in figure 7. Edge events therefore appear
 470 to be caused by fluorescence, where either an isolated or bipixel event becomes a tripixel
 471 due to the fluorescence photon. The distribution for centre events in contrast, shows that
 472 most (i.e. $\sim 86\%$) of the events' non-maximum pixels have lower energies around 3-5 keV
 473 – well below fluorescence energies. This suggests that centre events are predominately
 474 a result of charge spreading over to the adjacent pixels. The centre events distribution
 475 shows that some of the events are still due to fluorescence (i.e. the bright streaks), but
 476 at lesser rates than for edge events.

477 The distribution for the outer line events is most alike the edge events distribution,
 478 indicating that these events too are generally a consequence of fluorescence. Centre line
 479 events occur less frequently, making up 33% of all line events in the 59.5 keV experimental

480 data. Their distribution is more similar to that of right-angle centre events, suggesting
 481 more charge spreading in these events, although a larger proportion of counts result from
 482 fluorescence, with $\sim 29\%$ of counts in the fluorescence streaks when using a 1 keV energy
 483 window.

	Experiment (%)		Model (%)	
	59.5 keV	122 keV	59.5 keV	122 keV
Bipixels	12.4 ± 2.1	9.3 ± 1.9	11.8 ± 1.3	8.6 ± 1.2
Tripixels	61.1 ± 1.1	57.0 ± 2.5	65.4 ± 1.5	59.3 ± 2.0

Table 7: Percentage of bipixels and tripixels that are due to fluorescence as calculated experimentally and predicted by the model. The uncertainties were calculated from the difference when using a 1 keV and 2 keV energy window around the fluorescence spots/streaks.

484 By determining all edge and outer line events as resulting from fluorescence, and
 485 right-angle and line centre events from charge spreading (with the exception of the bright
 486 spots/streaks at 23 and 26 keV), the fraction of tripixels due to fluorescence was calcu-
 487 lated. Using the simulated data at 59.5 keV, the same analysis as for the experimental
 488 data was performed, also shown in figure 11 for comparison. The distributions from the
 489 modelled data show similar results. Since the model does not account for charge loss
 490 across the pixel gap, the curves in the edge and outer line event distributions are linear.
 491 Curves from the Cd K_β and Te K-shell fluorescence can therefore be resolved. For centre
 492 events, the model predicts that the energy shared amongst the non-maximum pixels is
 493 less concentrated at lower energies than the experimental data shows. Table 7 shows the
 494 portion of tripixels due to fluorescence from both experiment and model. The majority
 495 of tripixels appear to be a result of fluorescence, whereas bipixels are predominately due
 496 to charge spreading.

497 The 59.5 keV photopeak for the four different tripixel event types is shown in figure
 498 12. The peak position for the right-angle centre events is lower at 54.5 keV compared to
 499 the position for the edge and outer line event peaks at 56.5 keV. This again suggests that
 500 centre events are mostly due to charge spreading and not fluorescence as they exhibit
 501 more charge loss. When removing centre events from the tripixel photopeak, the peak
 502 FWHM improves from 5.1 keV to 4.6 keV.

Figure 12: ^{241}Am 59.5 keV tripixel photopeaks. (Top) photopeak for all tripixel events combined. (Middle) photopeak for outer line and edge tripixel events combined. (Bottom) Individual photopeak for each type of tripixel event. In all cases, the peaks have been normalised as a probability density function.

6. Conclusion

This paper described an end-to-end fully spectroscopic Monte-Carlo model which can simulate the spectral response of a pixelated CdTe detector.

The simulated spectra including isolated events only are in good agreement with experimental data taken with a 1 mm thick CdTe detector coupled to the HEXITEC ASIC, accurately predicting the CdTe escape peaks and fluorescence peaks, and the presence of a low energy tail due to charge trapping and noise thresholding.

High energy pixelated radiation detectors are known to exhibit large amounts of charge sharing which degrades their spectral performance. The model was able to estimate to a good degree the probability of charge sharing occurring at different energies. Given that the model could reproduce results seen experimentally, factors influencing charge sharing could be determined. This showed that the average charge cloud size is in fact relatively constant from 5-100 keV at $\sigma \approx 13 \mu\text{m}$ (a diameter of $\sim 78 \mu\text{m}$ to contain

516 $\sim 99.7\%$ of cloud charges), and that its final size is dominated by diffusion and electron
517 repulsion during drift as opposed to the initial cloud size. The noise threshold therefore
518 significantly reduces the amount of charge sharing at lower photon energies. The CdTe
519 absorption edges were found to have a significant impact on the proportion of shared
520 events.

521 Fluorescence shared events are characteristically different as they are not a result
522 of charges spreading across pixels, and therefore do not suffer from charge loss to the
523 inter-pixel region. The model was able to predict similar rates for the shared events due
524 to fluorescence as was measured experimentally. Understanding the different types of
525 shared events is critical for certain correction techniques such as the energy-loss correction
526 described in [12], which can currently only correct energy-loss in bipixel events but could
527 be expanded to include tripixels.

528 The model can be used to estimate the expected probability of charge sharing for
529 different sensor thicknesses, pixel sizes and operating voltages to inform detector design
530 depending on the desired application and energy range of interest. The next steps will
531 be to rigorously test the model with different input parameters when experimental data
532 for comparison is available. The model will also be extended to work with CdZnTe based
533 detectors. The effect of varying the noise threshold on the probability of charge sharing
534 will also be looked at closely.

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540 **Declaration of competing interest**

541 The authors declare that there are no known conflicts of interest associated with this
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543 **References**

- 544 [1] A. Owens, Compound semiconductor radiation detectors, 1st Edition, Taylor &
545 Francis Group, European Space Agency, Netherlands, 2012.
- 546 [2] P. Seller, S. Bell, R. Cernik, C. Christodoulou, C. Egan, J. Gaskin, S. Jacques, Pixel-
547 lated Cd(Zn)Te high-energy x-ray instrument, Journal of Instrumentation 6 (12)
548 (2012) 1–15.
- 549 [3] E. Goshen, L. Beilin, E. Stern, Feasibility study of a novel general purpose czts-based
550 digital spect camera: initial clinical results, EJNMMI Phys 14 (2018).
- 551 [4] A. Meuris, Semiconductor detector developments for high energy space astronomy,
552 Journal of Instrumentation 9 (2014).
- 553 [5] H. Barret, J. Eskin, Charge transport in arrays of semiconductor gamma-ray detec-
554 tors, Physical Review Letters 75 (1) (1995).
- 555 [6] A. Cola, I. Farella, The polarization mechanism in CdTe Schottky detectors, Applied
556 Physics Letters 94 (10) (2009) 1–4.
- 557 [7] W. Shockley, Currents to conductors induced by a moving point charge, Journal of
558 Applied Physics 10 (9) (1938) 635.
- 559 [8] M. Veale, S. Bell, D. Duarte, A. Schneider, P. Seller, M. D. Wilson, K. Iniewski,
560 Measurements of charge sharing in small pixel cdte detectors, Nuclear Instruments
561 and Methods in Physics Research A 767 (2014) 218–226.
- 562 [9] H. Iniewski, Modeling charge-sharing effects in pixellated czts detectors, Nuclear
563 Science Symposium Conference Record 6, 2007.
- 564 [10] A. Meuris, O. Limousin, C. Blondel, Charge sharing in cdte pixilated detectors,
565 Nuclear Instruments and Methods in Physics Research A 610 (1) (2009) 294–297.
- 566 [11] P. Zambon, V. Radicci, Spectral response characterization of cdte sensors of different
567 pixel size with ibex asic, Nuclear Inst. and Methods in Physics Research A 892 (2018)
568 106–113.

- [12] S. Bugby, K. Koch-Mehrin, M. Veale, J. Lees, Energy-loss correction in charge sharing events for improved performance of pixellated compound semiconductors, Nuclear Instruments and Methods in Physics Research A 940 (2019) 142–151.
- [13] L. Jones, P. Seller, M. Wilson, A. Hardie, Hexitec asic-a pixellated readout chip for czt detectors, Nuclear Instruments and Methods in Physics Research A 604 (1-2) (2009) 34–37.
- [14] <https://www.python.org/downloads/release/python-370/> (accessed on April 7th, 2020).
- [15] R. Evans, The Atomic Nucleus, 1st Edition, McGraw-Hill Book Company, Inc, New York, 1955.
- [16] M. Berger, J. Hubbell, S. Seltzer, J. Chang, J. Coursey, R. Sukumar, D. Zucker, K. Olsen, XCOM: Photon cross sections database, NIST, PML, Radiation Physics Division (1998) 87–3597.
- [17] M. Born, Atomic Physics, 8th Edition, Blackie and Sons, 1969.
- [18] R. Jenkins, Quantitative X-ray Spectrometry, 2nd Edition, Practical Spectroscopy volume 20, Marcel Dekker INC., New York, USA, 1995.
- [19] A. Compton, A quantum theory of the scattering of x-rays by light elements, Phys. Rev 21 (5) (1923) 483–502.
- [20] O. Klein, Y. Nishina, Über die streuung von strahlung durch freie elektronen nach der neuen relativistischen quantendynamik von dirac, Z. Phys. 52 (1929) 853–868.
- [21] A. Thompson, D. Attwood, X-Ray Data booklet, 3rd Edition, Center for X-ray Optics and Advanced Light Source, Berkeley, CA, 2009.
- [22] Kaye & Laby Online, Tables of Physical & Chemical Constants, <https://www.ase.org.uk/resources/kaye-and-laby-tables-physical-constants> (accessed on April 4th, 2020).
- [23] R. Redus, J. Pantazis, T. Pantazis, A. Huber, B. Cross, Characterization of CdTe detectors for quantitative X-ray spectroscopy, IEEE Transactions on Nuclear Science 56 (4) (2009) 2524–2532.

- [24] M. Benoit, L. Hamel, Simulation of charge collection processes in semiconductor
cdznte γ -ray detectors, Nuclear Instruments and Methods in Physics Research A
606 (3) (2009) 508–516.
- [25] P. Trueb, P. Zambon, C. Broennimann, Assessment of the spectral performance of
hybrid photon counting x-ray detectors, Medical Physics 44 (9) (2017) 207–214.
- [26] A. Fick, Ueber Diffusion, Annalen der Physik (1855).
- [27] A. Einstein, Über die von der molekularkinetischen theorie der wärme geforderte
bewegung von in ruhenden flüssigkeiten suspendierten teilchen, Annalen der Physik
332 (8) (1901) 549–560.
- [28] I. Blevis, R. Levinson, Photon-counting detectors and clinical applications in medi-
cal CT imaging, in: J. Iwanczyk (Ed.), Taylor & Francis Group, Oxford University
Press, 2005, Ch. 7, pp. 169–192.
- [29] K. Hecht, Zum mechanismus des lichtelektrischen primärstromes in isolierenden
kristallen, Zeitschrift für Physik A Hadrons and Nuclei 77 (1932) 235–245.
- [30] D. Duarte, J. Lipp, A. Schneider, P. Seller, M. Veale, M. Wilson, M. Baker, P. Sellin,
Simulation of active-edge pixelated cdte radiation detectors, Nuclear Instruments
and Methods in Physics Research A 806 (2016) 139–145.
- [31] M. Veale, S. Bell, P. Seller, M. Wilson, V. Kachkanov, X-ray micro-beam charac-
terization of a small pixel spectroscopic CdTe detector, Journal of Instrumentation
7 (7) (2012).
- [32] A. Cola, I. Farella, Electric field properties of CdTe nuclear detectors, IEEE Nuclear
Science Symposium Conference Record, 2006.
- [33] E. Kalemci, J. L. Matteson, Investigation of charge sharing among electrode strips
for a CdZnTe detector, Nuclear Instruments and Methods in Physics Research A:
478 (3) (2002) 527–537.
- [34] M. Veale, P. Seller, M. Wilson, E. Liotti, HEXITEC: A High-Energy X-ray Spec-
troscopic Imaging Detector for Synchrotron Applications, Synchrotron Radiation
News 31 (6) (2018) 28–32.

⁶²⁵ [35] Amptek, <https://www.amptek.com> (accessed on April 4th, 2020).