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Monte Carlo investigation of charge-transport effects on energy resolution and detection efficiency of pixellated CZT detectors for SPECT/PET applications

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Purpose: Semiconductor detectors are increasingly considered as alternatives to scintillation crystals for nuclear imaging applications such as positron emission tomography (PET) or single photon emission computed tomography (SPECT). One of the most prominent detector materials is Cadmium Zinc Telluride (CZT) which is currently used in several application-specific nuclear imaging systems. In this work, the charge transport effects in pixellated CZT detectors in relation to detector pixel size and thickness are investigated for pixels sizes from 0.4 up to 1.6 mm.

Methods: The determination of an optimum pixel size and thickness for use with photon energies of 140 and 511 keV, suitable for SPECT and PET studies, is attempted using photon detection efficiency and energy resolution as figures of merit. The Monte Carlo method combined with detailed finite element analysis was utilized to realistically model
photon interactions in the detector and the signal generation process. The Geant4 Application for Tomographic Emission (GATE) toolkit was used for photon irradiation and interactions simulations. The COMSOL Multiphysics® software application was used to create finite element models of the detector that included charge drift, diffusion, trapping and generation. Data obtained from the two methods were combined to generate accurate signal induction at the detector pixels. The energy resolution was calculated as the full width of half maximum of the energy spectrum photopeak. Photon detection efficiency was also calculated. The effects of charge transport within the detector and photon escape from primary pixel of interaction were investigated; the extent of diffusion to lateral pixels was also assessed.

Results: Charge transport and signal induction were affected by the position of a pixel in the detector. Edge and corner pixels were less susceptible to lateral diffusion than pixels located in the inner part of the detector. Higher detection efficiency and increased photon escape from primary interaction pixel were observed for thicker detectors. Energy resolution achieved better values in 0.7 and 1.0 mm pixel size for 5 mm detector thickness and 1.6 mm pixel size for 10 mm thickness.

Conclusions: Selection of pixel size and thickness depends on the imaging application and photon energy utilized. For systems that integrate two nuclear imaging modalities (i.e. combined SPECT/PET) the pixel size should offer an appropriate balance of the effects that take place in the detector, based on the results of the current work. This allows for a system to be designed with the same detector material and same geometrical configuration for both modalities.
I. INTRODUCTION

Nuclear medicine imaging systems are currently based on detectors manufactured using scintillation materials.\(^1\) However, dedicated systems employing semiconductor detectors based on cadmium zinc telluride (CZT) have already been introduced into clinical practice for breast and cardiac studies\(^2^7\) and demonstrated better image quality and sensitivity than conventional systems. Compared to other semiconductor materials, CZT is currently considered an attractive candidate for use in x- and gamma-ray imaging. It is a wide band-gap semiconductor with high effective atomic number (~60) and high density (~5.8 g/cm\(^3\)) that operates at room temperature without the need of cooling devices to maintain nominal operating conditions. Hence, its compact size and portability can be amply exploited to design dedicated and whole-body imaging systems.

The main advantage of semiconductor over scintillation detectors is their unique ability to directly convert the impinged photon energy to measured signal. Photons interact with the semiconductor and charge carriers (electron-hole pairs) are generated that move towards the detector electrodes under the influence of an externally applied electric-field. The number of generated carriers depends on the deposited energy and the average energy required to create one electron-hole pair in the detector material (4.64 eV for CZT). As long as the carriers are moving, signal is induced at the detector electrodes that can be measured using charge-sensitive amplifiers. In contrast, common scintillation detectors require more than one media to produce a measured signal. The generated carriers by the photon interaction are converted to light at luminescent centers within the scintillation crystal and the light is then converted to photoelectrons by the photocathode.
material. The photoelectron current is amplified in the photomultiplier to create the final signal. The whole signal generation process requires at least an order of magnitude more energy to create one carrier pair than in semiconductors, increasing the statistical noise to the measured signal that degrades the energy resolution of the system.\textsuperscript{1,8} The energy resolution in semiconductor detectors has been experimentally found\textsuperscript{9} better than what expected from the Poisson statistics in carrier generation. This was attributed to the inherent process of charge carrier generation in semiconductors and quantified by the Fano factor\textsuperscript{9} which adjusts for the deviation of the generated charge-carriers variance from Poisson statistics.

However, impurities and defects in the semiconductor material introduce new energy levels at which carriers are trapped along their drift. Due to carrier trapping, the induced signal depends on the photon interaction position. Signal dependence on the interaction position is observed in the energy spectrum through the “tail effect” of the photopeak, where a number of detected photons is incorrectly registered at lower energies instead of the photopeak.\textsuperscript{10} In compound semiconductors (such as CZT) the effect of trapping and the resultant degradation of photopeak efficiency are enhanced by lower mobility of both carrier types compared to elemental semiconductors, such as germanium or silicon. Holes are usually more severely affected since they have lower mobility than electrons. In addition, difficulties in manufacturing CZT detectors with high quality properties over large volumes prevent the production of detectors with thickness greater than 1 cm without a substantial increase in purchasing cost.

Single-polarity carrier sensing techniques\textsuperscript{11} were introduced to overcome the problem of severe trapping by rendering the detector nearly insensitive to drift of carriers with the
lower mobility. Barrett et al.\textsuperscript{12} demonstrated that detectors equipped with pixellated anode arrays\textsuperscript{13} and small pixel size, are almost insensitive to hole movement and improve energy resolution without sacrificing photopeak efficiency (small pixel effect). Nonetheless, later studies suggested that effects of photon scattering in the detector\textsuperscript{14} and charge sharing due to carrier diffusion in adjacent pixels\textsuperscript{15,16} lead to reduced photopeak efficiency and increased noise for very small pixels. Hence, proper selection of detector pixel size and thickness would allow better spatial and energy resolution of the imaging system without or with negligible compromise in its sensitivity. In a previous work from our team, Guerra et al.\textsuperscript{17} estimated that a detector with 1 mm pixel size and 6 mm thickness would attain reasonable detection efficiency in the range between 25 to 511 keV. They used a two-dimensional (2D) home-grown simulation application to investigate the detection efficiency and energy resolution of CZT detectors with different pixel sizes and thickness, focusing on the noise considerations of the read-out signal.

The purpose of the current work is to determine the optimum pixel size of pixellated CZT detectors for use in imaging applications that utilize 140 and 511 keV photons, based on the photopeak detection efficiency and energy resolution. Detailed and realistic three-dimensional models of the CZT detector were constructed using the COMSOL Multiphysics\textsuperscript{®} finite element method (FEM) software application and the Geant4 Application for Tomographic Emission\textsuperscript{18} (GATE) Monte Carlo method (MC) toolkit to obtain the induced signal at the electrodes and accurate photon interaction positions. Charge transport, trapping, diffusion and bias potential were implemented in the FEM models using the adjoint equation method described by Prettyman\textsuperscript{19} to obtain a map of the induced charge at the electrodes. The map was combined with photon interaction
positions obtained from the MC models for 140 and 511 keV photon irradiation. The combined output was used to calculate energy resolution and photopeak detection efficiency per pixel size and thickness.

II. METHODS

A. Signal induction modeling

1. Signal induction in semiconductors

Positron emission tomography (PET) and single-photon emission computed tomography (SPECT) applications utilize photons with energies in the region between 100 and 511 keV that interact with semiconductor materials mainly through photoelectric absorption and Compton scattering. The photon energy, or part of it in the case of Compton scattering, is transferred to an electron of the detector material; a small part is used to overcome the electron binding energy and the rest is given as kinetic energy. The free electron travels along the material in tortuous fashion caused by Coulomb interactions with orbital electrons and nuclei of the atoms until it completely loses its energy. Interactions with nuclei produce bremsstrahlung radiation due to the deceleration of the electron. Inelastic collisions with orbital electrons result in energy transfer and excitation of electrons to the conduction band and subsequent creation of holes in the valence band (electron-hole pairs). The number of charge-carriers generated along the path of the
primary electron is proportional to the energy of the incident photon $E_{ph}$ and depends on the average energy $w$ needed to excite electrons from valence to conduction band, which is a material property. We assumed a normal distribution $N$ of the carrier concentration $n$ around a mean value $\bar{n}$ with variance $\sigma^2$,

$$N \sim n\left(\frac{E_{ph}}{w}, \sigma^2 = F \cdot \frac{E_{ph}}{w}\right)$$  \hspace{1cm} (1)

where the Fano factor $F$ is not accurately known but several experiments have shown a value approximately equal to 0.1.\(^{20,21,22}\)

External application of electric field at the detector electrodes incites movement of the generated charge-carriers that drift towards electrodes with opposite sign. The electric field $\vec{E}$ and potential $\phi$ in the detector can be calculated using the Gauss's law and Poisson's equation for charge density $\rho$ and dielectric constant $\varepsilon$:

$$\nabla \vec{E} = \frac{\rho}{\varepsilon}$$  \hspace{1cm} (2)

$$\vec{E} = -\nabla \phi \rightarrow -\nabla^2 \phi = \frac{\rho}{\varepsilon}$$  \hspace{1cm} (3)

The drift velocity $\vec{v}$ of carriers depends on the electric field and the mobility $\mu$ of carriers, which is a property of the semiconductor material.\(^{23}\)

$$\vec{v} = \mu \cdot \vec{E}$$  \hspace{1cm} (4)

Electrons and holes usually have different mobility values in the same material and therefore a subscript is used to discriminate between electron $\mu_e$ and hole $\mu_h$ mobility. The current density $\vec{J}$ of drifting carriers with point charge $q$ is given by\(^{23}\)

$$\vec{J} = q \cdot (\mu_e \cdot n + \mu_h \cdot p) \cdot \vec{E}$$  \hspace{1cm} (5)
where \( n \) denotes the electron and \( p \) the hole concentration.

The generated electron-hole pairs are initially confined to the primary electron path and create a small area of high concentration of carriers within the detector. Due to random thermal motion and scattering they diffuse following the Fick’s law of diffusion and create a flux of carriers towards areas of low concentration. In the current study only electrons were considered and therefore the rest of the equations will refer to electrons only. However similar equations apply to holes. The current density of electron diffusion \( \vec{J}_{\text{D}_n} \) is given by

\[
\vec{J}_{\text{D}_n} = D_n \cdot \nabla n
\]  

(6)

The diffusion constant for electrons \( D_n \) is connected to individual detector materials through the Einstein relation

\[
D_n = \frac{k \cdot T}{q \cdot \mu_n}
\]  

(7)

where \( k \) is the Boltzmann constant and \( T \) the absolute temperature. In detectors with pixellated electrode configuration, charge carriers generated in the area between two pixels can diffuse and be collected by two different pixels leading to charge sharing, and hence reduced charge collection by individual electrodes. The current-density equation for electrons, \( \vec{J}_n \), consists of both drift [Eq. (5)] and diffusion [Eq. (6)] components

\[
\vec{J}_n = q \cdot (\mu_n \cdot n \cdot \vec{E} + D_n \cdot \nabla n) = -q \cdot (\mu_n \cdot n \cdot \nabla \phi - D_n \cdot \nabla n)
\]  

(8)

The number of carriers finally reaching the electrodes is different from the one initially generated by photon interactions, due to carrier diffusion, previously described, and carrier trapping at energy levels introduced by impurities and defects of the material. Each carrier type is associated with an average lifetime \( \tau \) before trapping. The trapping
rate for electrons is given by

$$U_n = \frac{n}{\tau_e} \quad (9)$$

where $\tau_e$ is the average lifetime of electrons.

Carrier concentration in the detector along time can be calculated using the continuity equation. For electrons the continuity equation becomes

$$\frac{\partial n}{\partial t} = G_n - \frac{n}{\tau_e} - \mu_e n \nabla \phi + D_e \nabla n \quad (10)$$

where $G_n$ is the carrier generation term. This term is set equal to the Dirac's delta function to obtain the concentration of an impulse charge

$$G_n = \delta(\vec{r} - \vec{r}_0) \cdot \delta(t) \quad (11)$$

where $\vec{r}_0$ is the initial position of the charge carrier.

Throughout the carrier movement within the detector volume, mirror charges are induced at the electrodes until all carriers are fully collected. The induced charge (signal) per unit time can be measured using suitable read-out electronics to estimate the initial photon energy.

Calculation of the signal was made using the Shockley-Ramo theorem. The theorem introduced the concept of weighting field $\vec{E}_w$ and its weighting potential $\phi_w$ to obtain the current $i$ and charge $q_{ind}$ induced at an electrode by a moving carrier. The weighting field is the field that would exist at a moving carrier position if all other charges were removed, the selected electrode had unit potential and all other electrodes were earthed. The weighting potential could be calculated from the Poisson equation similarly to Eq. (3). The shape of the weighting potential in pixellated detectors is
depicted in Fig. 1 where the $\phi_w$ across the detector at the middle of a pixel with 1 mm size and the 2D spatial distribution are shown. From the Shockley-Ramo theorem the induced charge along the weighting potential of Fig. 1b would be given by

$$q_{\text{ind}} = -q \cdot (\phi_w(x_a) - \phi_w(x_0)),$$

where $\phi_w(x_a)$ is the weighting potential in the collecting anode and $\phi_w(x_0)$ is the weighting potential at the electron generation location ($x_0$). Small pixels have a region in the vicinity of the anode where the weighting potential has a steep rise (Fig. 1b). If a photon interacts within this region, the difference between the weighting potentials in the electron generation location and the collecting anode will be much less than one and the induced charge will be less than that induced from other parts of the pixel volume. Hence, reduced charge induction is also associated with depth of photon interaction when this is in the vicinity of the anode.

The induced charge due to electron movement along the detector for time $t'$, is obtained through

$$q_{\text{ind}} = q \cdot \int_0^{t'} \int_{\Omega} \mu \cdot n(\vec{r}, t) \cdot \nabla \phi_w \cdot \nabla \phi_w \cdot d^3r$$  \hspace{1cm} (12)

where $\Omega$ defines all points in the volume of the detector (or pixel), and $n(\vec{r}, t)$ is calculated from Eq. (10).

The charge induction efficiency (CIE), $\eta_k$, of the $k$ electrode for a specific position in the detector gives the shape of the pulse arising due to a charge generation at that location. It is calculated as the ratio of the induced charge to the initial charge

$$\eta_k = \frac{q_{\text{ind}}}{q}.$$  \hspace{1cm} (13)

Calculation of CIE using Eqs. (3), (10), (11) and (12) for all possible interaction
locations in a detector, requires unrealistic amount of time and effort. Prettyman\textsuperscript{19, 24} suggested a method to obtain a map of the CIE along time for all possible interaction positions using the adjoint electron $n^*$ continuity equation

$$\frac{\hat{c}n^*}{\hat{c}t} = \mu_e \nabla \phi \nabla \phi_e - \frac{n^*}{\tau_e} + \mu_e \nabla \phi \nabla n^* + D_e \nabla^2 n^*. \quad (14)$$

The generation term [Eq. (12)] in Eq. (11) is substituted with the adjoint electron generation term

$$G_{n^*} = \mu_e \nabla \phi \nabla \phi_e \quad (15)$$

The solution of Eq. (14) is the CIE as given by Eq. (13) but for all possible interaction positions in the detector. This CIE map can be used to estimate the induced signal at the anodes from energy deposition of a photon interaction.

2. Finite Element Models

Charge transport in the detector module was modeled with FEM using the COMSOL Multiphysics\textsuperscript{®} software application. The software provided graphical user interface to define the geometry of the model and its environment, specify material properties and physical constants, and implement the necessary equations [Eqs. (3), (14) and (15)] that describe the physical processes. Carrier mobility, dielectric constant and other CZT material properties were acquired from EI Detection & Imaging Systems (http://www.evmicroelectronics.com) and presented in Table I.

The detector modules were comprised by 16 pixels in four by four square pixel
arrangement. CIE maps were generated for modules with pixel size equal to 0.4, 0.7, 1.0, 1.3, and 1.6 mm and two thicknesses, 5 and 10 mm. The bias potential between the anode and the cathode in the FEM models was -900 V for the 5 mm and -3600 V for the 10 mm detector thickness. All FEM models employed ohmic contacts. Pixels located at the edge, corner and inner part of the module were separately modeled and the CIE was computed for each one. Cross-sections along the detector thickness were obtained to assess the CIE along depth.

255 B. Monte Carlo simulations

Models of CZT detectors were created using the Geant4 application for tomographic emission\textsuperscript{18} (GATE), a well-validated code for nuclear-medicine imaging applications. The detectors were composed of modules with 256 pixels in 16 by 16 square pixel arrangement. Pixel size and thicknesses of the MC models corresponded to the pixel size and thickness used in the FEM models. The number of modules in each detector varied according to the pixel size. The overall lateral detector dimensions were 200 by 200 mm\textsuperscript{2}. Pixel separation was 0.1 mm and module separation was 0.3 mm. Point sources emitting photons with 140 and 511 keV energy at 10 cm distance from the detector face were modeled. Source activity was set to 37 MBq and the detector was separately irradiated by each source until the number of detected photons in each detector was in the order of 10\textsuperscript{6}. Photons entered the detector from the cathode side. Photoelectric effect, Compton and Rayleigh scattering as well as x-ray fluorescence were included in the models.
C. Calculations

The volume affected by the depth of interaction, $V_{\text{depth}}$, was determined as a parallelepiped with base equal to pixel size squared and height given by the distance from anode after which the value of CIE across the detector thickness drops below 0.9. This is approximately the depth near the vicinity of the anode at which the CIE starts to drop and the weighting potential starts to rise as shown in Fig.1. The ratio of $V_{\text{depth}}$ to total pixel volume, $V_{\text{pixel}}$, was calculated as

$$R_{\text{depth}} = \frac{V_{\text{depth}}}{V_{\text{pixel}}}.$$  \hspace{1cm} (16)

The CIE gradient across the pixel width was also obtained to estimate the charge-carrier diffusion length, $L$, within the pixel volume. The ratio of the pixel volume affected by diffusion, $R_{\text{diff}}$, to the total pixel volume was calculated by

$$R_{\text{diff}} = \frac{V_{\text{diff}}}{V_{\text{pixel}}}.$$  \hspace{1cm} (17)

Diffusion volume, $V_{\text{diff}}$, is the volume of the pixel where the induced signal from an energy deposition will be affected by charge diffusion. The charge-carrier diffusion length changes with depth and hence it can be approximated as the complement of a trapezoid that extends across the pixel, with the large base at anode and small base at the cathode. Calculation of the diffusion volume is made by subtraction of a trapezoid volume from the pixel volume.
\[ V_{\text{diff}} = d \cdot p^2 - \frac{1}{2} \cdot d \cdot \left[ p^2 + (p - L)^2 \right] \]  

(18)

where \( d \) is the pixel thickness and \( p \) the pixel size.

When small pixel sizes are utilized there is an increased probability that a photon will escape the pixel volume of its primary interaction. The escape photon can either be detected by neighboring pixels or completely escape the detector volume. This is detrimental to the photopeak efficiency since it removes counts that would otherwise have been registered in the photopeak. In the current work, the notation \( N_{\text{esc}} \) is used to represent the counts from photons that interacted with and escaped from their primary pixel volume and detected by neighboring pixels. The total number of counts registered in the whole detector is denoted with \( N_{\text{tot}} \). One count is the pulse arising at one pixel using basic read-out electronic as described in GATE. Energy depositions from the same photon in the same pixel are summed to create one pulse. The escape ratio, \( R_{\text{esc}} \), was then defined as

\[ R_{\text{esc}} = \frac{N_{\text{esc}}}{N_{\text{tot}}} \]  

(19)

The counts from photons that deposit all their energy in the volume defined by one pixel are denoted as \( N_{\text{full}} \) and the full-energy ratio \( R_{\text{full}} \) as

\[ R_{\text{full}} = \frac{N_{\text{full}}}{N_{\text{tot}}} \].  

(20)

The term \( R_{\text{esc}} \) does not include photons that scattered and completely escaped the detector; hence the sum of \( R_{\text{esc}} \) and \( R_{\text{full}} \) will be less than unity.
Due to the dependence of the CIE to the interaction position the counts from photons that generate a signal high enough to be registered in the photopeak, \( N_{\text{peak}} \), will be less than the \( N_{\text{full}} \). The photopeak ratio, \( R_{\text{peak}} \), was defined as

\[
R_{\text{peak}} = \frac{N_{\text{peak}}}{N_{\text{full}}}. \tag{21}
\]

The closer the value of \( R_{\text{peak}} \) is to one the less is the effect of charge transport on the photopeak efficiency.

The broadening of energy spectrum due to charge transport effects and quantum statistics is assessed using the energy resolution \( R_{\text{FWHM}} \). \( R_{\text{FWHM}} \) was obtained from the full width at half maximum (FWHM) of the photopeak in the energy spectrum divided by the peak-energy, \( E_{\text{peak}} \),

\[
R_{\text{FWHM}} = \frac{\text{FWHM}}{E_{\text{peak}}}. \tag{22}
\]

III. RESULTS

The cathode potential in the FEM models was equal to -900 V and -3600 V for 5 and 10 mm detector thickness respectively. These values were selected because they better compensate for trapping effects. In Fig. 2, the CIE curve for 0.7 mm pixel size and 5 mm thickness is shown at different cathode potential values. Higher potential resulted in less slope of the linear part of CIE curve. At -900 Volts, CIE was approximately constant along most of pixel depth. Similar curves were obtained for all pixels sizes at 5 and 10 mm thickness. Change in pixel size and lateral detector dimensions did not affect the
value of cathode potential at which better trapping compensation was achieved because electrons drifted along the electric field gradient that existed between the anode and the cathode.

Charge induction efficiency for inner, edge and corner pixels is presented in Fig. 3 for 1 mm pixel size and 10 mm thickness. Pixels located at the corners and edges of the 4 by 4 pixel detector module presented smoother curve near the collection anode. Pixels located at the inner part of the module had approximately constant value of CIE at greater depth in the pixel. In Table II, the difference between the maximum CIE value and the value at distance from anode equal to the pixel size and twice the pixel size is presented for pixels with 5 mm thickness. Similar calculation were performed for 10 mm thickness and presented in Table III. The maximum value of CIE for each pixel was between 0.9 and 0.934. The depth at which the CIE value dropped below 0.9 is presented in Table IV. If two interactions occurred at different depths after this point and deposited the same energy, the induced charge from each interaction would be different due to the fast decrease of CIE near the anode, and the tail effect would be observed in the energy spectrum.

Figure 4, shows the CIE curve for different pixel sizes with 5 mm thickness. The CIE value in smaller pixel sizes decreased faster in the vicinity of the anode and maintained a constant value in the rest of the pixel depth. The same pattern was found for pixels with 10 mm thickness. In Fig. 5, the ratio of pixel volume affected by depth of interaction to the total pixel volume is presented for each pixel size and thickness. The fraction of pixel volume affected by interactions occurring near the anode increased with increasing pixel size.
In Fig. 6a, a cross-section of the 3D CIE map along the pixel thickness for 1 mm pixel size and 5 mm thickness is shown. Figure 6b, presents the CIE along the pixel width, obtained from the 2D slice, depicted in Fig. 6a. The extent of lateral diffusion was obtained from the CIE gradient near the junction between two pixels. Similar plots were constructed for each pixel and the volume affected by diffusion was calculated and presented in Fig. 7. The diffusion extent was found equal to 100 μm near the cathode for 5 mm pixel thickness and 150 μm for 10 mm. Near the anodes, lateral diffusion extended as little as 20 μm since electrons generated close to anodes are collected faster and they drifted for less time in the detector. The fraction of the pixel volume affected by diffusion extent was larger in smaller pixel sizes, since the extent itself was not affected by the lateral dimensions of the pixel.

The escape ratio is depicted in Fig. 8. More photons appear to escape the primary pixel and detected by neighboring pixels when smaller pixels were used. This however is not due to an actual increase in the number of scattered photons. It is rather attributed to an increased probability of a photon to escape the primary pixel of interaction when smaller pixels are used. There was less than 8% relative difference between the escape ratio for 5 and 10 mm thickness at 140 keV. However, at 511 keV, there was more than 18% relative difference between escape ratios for each thickness.

Figure 9, shows the full energy ratio, $R_{\text{full}}$. More photons deposited all their energy in one pixel volume when larger pixels were employed. In these calculations, the effect of depth of interaction and diffusion was not taken into account. The photopeak ratio, $R_{\text{peak}}$, quantified the effect of depth of interaction, diffusion, and trapping on photopeak detection. The CIE that inherently incorporated these effects was combined with the
energy deposited from each photon interaction to calculate the induced signal. Since trapping was compensated by potential, the effects could be attributed only to depth of interaction and diffusion. Values of $R_{\text{peak}}$ approximately equal to one indicate that photopeak efficiency was less affected by the aforementioned processes. Results for $R_{\text{peak}}$ and $R_{\text{full}}$ are presented in Table V.

The photon interaction position and the number of interactions at each position, for photons depositing their full energy in one pixel, are depicted in Fig. 10. Each column of the figure represents a pixel size. The effects of photon escape, diffusion, and depth of interaction on different pixel sizes are shown in the second row (Fig. 10b). The first row (Fig. 10a) depicts the number of interactions across the pixels including only photon escape information as obtained solely from Monte Carlo simulations.

Energy resolution was calculated from spectra obtained using the CIE information from FEM models and the results are shown in Table VI. The photopeak broadening was only attributed to quantum statistics from the initial number of charge-carriers generated by photon interactions and reduced induction signal due to charge diffusion and interactions near the anode.

IV. DISCUSSION

Geometrical constraints on the design of detector modules were important since pixels located at different positions in the module had different CIE characteristics (Fig. 3, Table II – IV). Pixels located at the inner part of the module had constant CIE for longer part of the detector thickness than pixels located at the edge or corner of the module. In contrast,
inner pixels were more susceptible to carrier diffusion since they were in contact with eight pixels instead of five and three pixels as in the case for edge and corner locations respectively. Hence, there were fewer pixels into which carriers could diffuse. Carrier diffusion had also stronger effect on smaller pixels. The diffusion length was found to be as much as 100 µm at the cathode side for 5 mm pixel thickness and 150 µm for 10 mm, close to the values reported by Kalemci et al.\textsuperscript{16} and He et al.\textsuperscript{15} The fraction of pixel volume affected by diffusion increased with decreasing pixel size. In the vicinity of the junction between pixels the CIE gradually decreased up to a distance defined by the diffusion extent, leading to misplaced counts in the energy spectrum. However, CIE remained constant in greater depth within smaller pixels (Fig. 4) and hence the small pixels were less affected by depth of photon interaction, particularly in the case of 511 keV photons that interacted deeper into the crystal.

As the pixel size decreased more counts were registered to the detector. This was attributed to an increased number of photons escaping the primary pixel of interaction and detected by neighboring pixels at smaller pixel sizes which was in accordance with the findings of Wagenaar et al.\textsuperscript{14} Photons escaping the primary pixel contributed more than 25% and 40% to the total registered counts for 140 and 511 keV respectively at 0.4 mm. Each pixel in semiconductor detectors was separately read by the read-out electronics and therefore energy deposited in two different pixels was not summed. This led to unwanted characteristic x-ray escape peaks that otherwise would have been registered at the photopeak and hence loss of useful information. The loss of photopeak information was related to the decreased number of photons that deposited their full energy in one pixel as the pixel size became smaller. A photon interacting with the
material and escaped to more than one pixel would have been detected as individual count at each pixel and not registered properly at the photopeak.

The full-energy ratio, $R_{\text{full}}$ and the photopeak ratio $R_{\text{peak}}$ were affected by: a) photon energy; since higher energy results in more scatter (Fig. 8) and less photons deposit all their energy in one pixel (Fig. 9). Higher energy photons are also more penetrating and more susceptible to interact near the anode and induce less signal. b) detector thickness; thicker pixels allow for longer electron drift and more volume to diffuse in (Fig. 7). c) pixel size; smaller pixel sizes are more susceptible to charge diffusion and photon escape (Fig. 7, 8). The photopeak ratio was a measure of the effects of diffusion and depth of interaction on photopeak detection (Table V). At 140 keV photons, carrier diffusion was more important since more than 70% of the interactions occurred at the first 2.5 mm and smaller pixels registered fewer counts in the photopeak. The fraction of photons escaping the primary pixel was more important also at smaller pixel sizes (Fig. 8). Depth of interaction becomes important after 1.3 mm pixel size, where the detected photons ratio starts to drop. $R_{\text{full}}$ was maximized at 1 mm pixel size for 5 mm detector thickness and 1.6 mm pixel size for the 10 mm thickness. At 511 keV, the effect of photons escaping the primary pixel and depth of interaction was more intense than in 140 keV. However, counts from photons escaping the primary pixel accounted for more than 30% of the total counts at 5 mm and 40% at 10mm thickness. Hence, at 5 mm thickness and 1 mm pixel size, approximately 10% of the incoming photons deposited all their energy in one pixel. The balance between diffusion, depth of interaction and photons escaping the primary pixel allowed the registration of more than 70% of them in the photopeak window. At 10 mm thickness, the variation of $R_{\text{full}}$ between different pixel sizes was small. For 1.6 mm
pixel size, ~10% of the detected photons deposited all their energy and more than 80% of them were registered in the selected photopeak window. The escape ratio reached its lowest value in this pixel size as well.

V. CONCLUSION

In the current study we attempted to estimate an optimum pixel size for CZT detectors with 5 and 10 mm thickness, suitable for imaging applications utilizing 140 and 511 keV photons. Photon scattering or escaping the primary pixel within the detector, carrier transport effects, photon detection and energy resolution were utilized as figures of merit. Their values were obtained from detailed three dimensional models of detectors, designed with the finite element method, and associated photon interactions implemented with the Monte Carlo method. Electron transport, trapping, diffusion and generation were included in the models. Photoelectric effect, Compton and Rayleigh scattering, and Coulomb interactions of electrons were also considered.

Pixel sizes less than 1 mm were affected more by inter-pixel scatter (or escape) and diffusion while larger pixel sizes were affected more by depth of interaction. At 140 keV photon energy, the best energy resolution was obtained at 0.7 mm for 5 mm thickness at the cost of reduced photon detection. Increase of pixel thickness provided better energy resolution at 1.6 mm pixel size and better detection but the manufacturing cost of a high quality detector with larger thickness is an issue to be considered. At 511 keV, the best energy resolution for 5 mm detector thickness was observed in 1 mm pixel size. Increase to 10 mm thickness provided better energy resolution and better photon detection at 1.6
mm pixel size but fewer photons were registered in the photopeak due to increased
scattering between pixels.

The selection of pixel size and thickness relies on the imaging application requirements
and the utilized photon energy. However, proper selection of pixel size and thickness
depending on the balance between the effects that take place within the detector could
allow optimum detector performance; specifically when systems that combine more than
one imaging modalities that operate in different photon energies come into consideration.
Proper balance between charge transport effects, detection efficiency and photon escape
from the primary pixel within the detector could be achieved using the results of the
current work for both 5 and 10 mm thickness. This could allow the integration of
PET/SPECT systems using the same detector material and geometrical configuration. The
performance of such systems is currently under investigation by the authors of the current
work, using the same modeling method.

In the current work, the contribution of holes was not considered due to the small pixel
effect\textsuperscript{12} and therefore transport phenomena for holes were not modeled. Further
improvements include the modeling of realistic read-out electronics that would account
for noise, dead time and coincidence timing and allow the design of realistic models of
PET and SPECT systems. In addition, modeling of charge sharing between adjacent
pixels could be improved by using spherical or ellipsoid charge-carrier cloud distribution
at each electron interaction instead of a point-like, used in this study. Using our modeling
method, thicker CZT detectors and more complicated multimodal PET/SPECT systems
for use in application-specific or whole-body imaging could be designed and
investigated.
ACKNOWLEDGMENTS

This work was supported by the Faringdon Proof of Concept Fund. We also acknowledge NHS funding to the NIHR Biomedical Research Centre of Excellence.
REFERENCES


7. D-SPECT™ Cardiac Imaging System Spectrum Dynamics.


W. Shockley, “Currents to Conductors Induced by a Moving Point Charge,” J. Appl. Phys. 9, 635 (1938).

FIG. 1. Weighting potential in pixellated detectors. The figure refers to 1 mm pixel size. On the left, the 2D distribution of the weighting potential is depicted. On the right, the weighting potential along a line crossing the detector at 0 mm is shown.
FIG. 2. Charge induction efficiency curves obtained from -200, -500, -700, and -900 V detector bias potential. The results shown were obtained from $0.7 \times 0.7 \times 5.0 \text{ mm}^3$ pixel size. Low bias potential resulted in non-constant CIE for most of the detector depth, increasing the “tail effect”.

FIG. 3. Charge induction efficiency for pixels located at the corner, edge and the inner part of the detector module. The CIE remained constant within larger depths for inner pixels. The results shown were obtained from pixels with dimensions equal to $1.0 \times 1.0 \times 10.0$ mm$^3$. The bias potential is -3600 V.
FIG. 4. CIE acquired from 0.4, 0.7, 1.0, 1.3, and 1.6 mm pixel sizes and 5 mm thickness. Smaller pixel sizes were less affected by depth of interaction. The detector was irradiated from the cathode side. The bias potential was -900 V.
FIG. 5. Ratio of the pixel volume affected by reduced charge induction efficiency to the total pixel volume for photons interacting close to anode.
FIG. 6. a) Two-dimensional cross section of CIE along the pixel. b) CIE across pixel width, obtained along the line depicted with purple color in 6a. The cross-section is taken at the center of the pixel with respect to the third dimension.
FIG. 7. Ratio of pixel volume where the CIE will be reduced due to charge diffusion to adjacent pixels to the total pixel volume.
FIG. 8. Escape ratios of photons interacting with 5 and 10 mm detector thickness and 0.4, 0.7, 1.0, 1.3, and 1.6 mm pixel size for a) 140 keV and b) 511 keV photon energy.
FIG. 9. Ratio of photons that deposit their full energy to the total pixel volume for pixel volumes with 5 and 10 mm thickness and a) 140 keV and b) 511 keV photon energy.
FIG. 10. Two-dimensional interaction maps that include the effects of photon escape from the primary pixel, diffusion and depth of interaction. A direct comparison of each effect on different pixel sizes is possible. At the first row (a), the pixels modelled only using Monte Carlo code are depicted. At the second row (b), FEM modelling is also included. Each column corresponds to a pixel size. The impact of diffusion and photon escape is greater in smaller pixels than in larger pixels where depth of interaction becomes dominant. Diffusion, depth of interaction and photon escape from the pixel can be observed. Interactions near 0 mm are in the vicinity of the cathode. The colormap decodes the number of interactions.
Table I. CZT material properties.

<table>
<thead>
<tr>
<th>CZT material properties</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Average atomic number</td>
<td>49.1</td>
</tr>
<tr>
<td>Density (g/cm³)</td>
<td>5.78</td>
</tr>
<tr>
<td>Band gap (eV)</td>
<td>1.572</td>
</tr>
<tr>
<td>Dielectric constant</td>
<td>10.9</td>
</tr>
<tr>
<td>Pair creation energy (eV)</td>
<td>4.64</td>
</tr>
<tr>
<td>Resistivity (Ωcm)</td>
<td>3x10^{10}</td>
</tr>
<tr>
<td>Electron mobility (cm²/Vs)</td>
<td>1000</td>
</tr>
<tr>
<td>Electron lifetime (s)</td>
<td>3x10^{-6}</td>
</tr>
<tr>
<td>Hole mobility (cm²/Vs)</td>
<td>50-80</td>
</tr>
<tr>
<td>Hole lifetime (s)</td>
<td>10^{-6}</td>
</tr>
</tbody>
</table>
Table II. CIE difference between the maximum value and the value at distances equal to the pixel size and twice the pixel size from anode for 5 mm pixel thickness.

<table>
<thead>
<tr>
<th>5 mm thickness</th>
<th>Distance from anode</th>
<th>1 x pixel size</th>
<th>2 x pixel size</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Pixel size (mm)</td>
<td>Inner pixel</td>
<td>Edge pixel</td>
</tr>
<tr>
<td>0.4</td>
<td>0.079</td>
<td>0.129</td>
<td>0.205</td>
</tr>
<tr>
<td>0.7</td>
<td>0.082</td>
<td>0.132</td>
<td>0.210</td>
</tr>
<tr>
<td>1.0</td>
<td>0.081</td>
<td>0.133</td>
<td>0.213</td>
</tr>
<tr>
<td>1.3</td>
<td>0.081</td>
<td>0.135</td>
<td>0.212</td>
</tr>
<tr>
<td>1.6</td>
<td>0.084</td>
<td>0.133</td>
<td>0.207</td>
</tr>
</tbody>
</table>
Table III. CIE difference between the maximum value and the value at distances equal to the pixel size and twice the pixel size from anode for 10 mm pixel thickness.

<table>
<thead>
<tr>
<th>Pixel size (mm)</th>
<th>Distance from anode</th>
<th>1 x pixel size</th>
<th>2 x pixel size</th>
</tr>
</thead>
<tbody>
<tr>
<td>10 mm thickness</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.4</td>
<td>0.088</td>
<td>0.132</td>
</tr>
<tr>
<td></td>
<td>0.7</td>
<td>0.085</td>
<td>0.137</td>
</tr>
<tr>
<td></td>
<td>1.0</td>
<td>0.085</td>
<td>0.137</td>
</tr>
<tr>
<td></td>
<td>1.3</td>
<td>0.084</td>
<td>0.135</td>
</tr>
<tr>
<td></td>
<td>1.6</td>
<td>0.083</td>
<td>0.134</td>
</tr>
</tbody>
</table>
Table IV. The depth at which CIE value becomes less than 0.9 for each pixel size and thickness.

<table>
<thead>
<tr>
<th>Pixel size (mm)</th>
<th>Distance from cathode (mm)</th>
<th>5 mm thickness</th>
<th>10 mm thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Inner pixel</td>
<td>Edge pixel</td>
<td>Corner pixel</td>
</tr>
<tr>
<td>0.4</td>
<td>4.43</td>
<td>4.20</td>
<td>3.95</td>
</tr>
<tr>
<td>0.7</td>
<td>4.00</td>
<td>3.60</td>
<td>3.15</td>
</tr>
<tr>
<td>1.0</td>
<td>3.55</td>
<td>3.00</td>
<td>2.40</td>
</tr>
<tr>
<td>1.3</td>
<td>3.12</td>
<td>2.44</td>
<td>1.76</td>
</tr>
<tr>
<td>1.6</td>
<td>2.72</td>
<td>2.00</td>
<td>1.30</td>
</tr>
</tbody>
</table>
Table V. $R_{\text{full}}$ and $R_{\text{peak}}$. A high photopeak ratio, $R_{\text{peak}}$, denotes that the pixel is less affected by depth of interaction and diffusion.

<table>
<thead>
<tr>
<th>Pixel size (mm)</th>
<th>140 keV</th>
<th>511 keV</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$R_{\text{full}}$</td>
<td>$R_{\text{peak}}$</td>
</tr>
<tr>
<td>0.4</td>
<td>0.48</td>
<td>0.65</td>
</tr>
<tr>
<td>0.7</td>
<td>0.59</td>
<td>0.76</td>
</tr>
<tr>
<td>1.0</td>
<td>0.65</td>
<td>0.78</td>
</tr>
<tr>
<td>1.3</td>
<td>0.70</td>
<td>0.76</td>
</tr>
<tr>
<td>1.6</td>
<td>0.73</td>
<td>0.74</td>
</tr>
</tbody>
</table>
Table VI. Energy resolution for 140 and 511 keV photons for different pixel sizes and thicknesses.

<table>
<thead>
<tr>
<th>Pixel size (mm)</th>
<th>140 keV</th>
<th>511 keV</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>5 mm</td>
<td>10 mm</td>
</tr>
<tr>
<td>0.4</td>
<td>1.54</td>
<td>2.31</td>
</tr>
<tr>
<td>0.7</td>
<td>1.08</td>
<td>1.53</td>
</tr>
<tr>
<td>1.0</td>
<td>1.15</td>
<td>1.42</td>
</tr>
<tr>
<td>1.3</td>
<td>1.46</td>
<td>1.23</td>
</tr>
<tr>
<td>1.6</td>
<td>1.54</td>
<td>1.15</td>
</tr>
</tbody>
</table>