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Andrey Makeev
Martin Clajus
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Andrey Makeev,^{a,*} Martin Clajus,^b Scott Snyder,^b Xiaolang Wang,^c and Stephen J. Glick^a

^aUniversity of Massachusetts Medical School, Department of Radiology, 55 Lake Avenue North, Worcester, Massachusetts 01655, United States

^bNOVA R&D, Inc., 833 Marlborough Avenue #200, Riverside, California 92507, United States

^cToshiba Medical Research Institute USA, Inc., 706 North Deerpath Drive, Vernon Hills, Illinois 60061, United States

Abstract. Semiconductor photon-counting detectors based on high atomic number, high density materials [cadmium zinc telluride (CZT)/cadmium telluride (CdTe)] for x-ray computed tomography (CT) provide advantages over conventional energy-integrating detectors, including reduced electronic and Swank noise, wider dynamic range, capability of spectral CT, and improved signal-to-noise ratio. Certain CT applications require high spatial resolution. In breast CT, for example, visualization of microcalcifications and assessment of tumor microvasculature after contrast enhancement require resolution on the order of 100 μm . A straightforward approach to increasing spatial resolution of pixellated CZT-based radiation detectors by merely decreasing the pixel size leads to two problems: (1) fabricating circuitry with small pixels becomes costly and (2) inter-pixel charge spreading can obviate any improvement in spatial resolution. We have used computer simulations to investigate position estimation algorithms that utilize charge sharing to achieve subpixel position resolution. To study these algorithms, we model a simple detector geometry with a 5×5 array of 200 μm pixels, and use a conditional probability function to model charge transport in CZT. We used COMSOL finite element method software to map the distribution of charge pulses and the Monte Carlo package PENELOPE for simulating fluorescent radiation. Performance of two x-ray interaction position estimation algorithms was evaluated: the method of maximum-likelihood estimation and a fast, practical algorithm that can be implemented in a readout application-specific integrated circuit and allows for identification of a quadrant of the pixel in which the interaction occurred. Both methods demonstrate good subpixel resolution; however, their actual efficiency is limited by the presence of fluorescent *K*-escape photons. Current experimental breast CT systems typically use detectors with a pixel size of 194 μm , with 2×2 binning during the acquisition giving an effective pixel size of 388 μm . Thus, it would be expected that the position estimate accuracy reported in this study would improve detection and visualization of microcalcifications as compared to that with conventional detectors. © 2015 Society of Photo-Optical Instrumentation Engineers (SPIE) [DOI: 10.1117/1.JMI.2.2.023501]

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1 Introduction

Most existing computed tomography (CT) detectors operate in an energy integrating mode, whereby images are formed by acquiring x-ray events over a finite acquisition time. For several reasons the performance of energy integrating detectors is sub-optimal for use in CT. A number of researchers have been investigating the use of direct conversion pixellated cadmium zinc telluride (CZT) or cadmium telluride (CdTe) semiconductor detectors that operate in a photon-counting mode.^{1–3} Photon-counting detectors for x-ray CT provide advantages over conventional energy-integrating detectors, including reduced electronic noise, wider dynamic range, capability of material decomposition, and improved signal-to-noise ratio through energy weighting. Certain CT applications such as small animal imaging, high-resolution volume-of-interest spectral CT, and breast CT would benefit from high-resolution photon-counting detectors. For example, in breast CT, visualization of tumor microvasculature and small microcalcifications is critical to

maximizing diagnostic performance and requires high spatial resolution. Preliminary patient studies with breast CT have suggested improved visualization of masses as compared to conventional mammography; however, the visualization of lesions exhibiting microcalcifications as compared to mammography is uncertain. Visualizing microcalcifications in x-ray breast imaging systems is important for the detection of ductal carcinoma *in situ* (DCIS). It has been estimated that DCIS represents 20% to 30% of all breast cancers detected in a screening program.⁴ Since at least 30% to 50% of all DCIS eventually become invasive if not treated,⁴ early detection and diagnosis of DCIS probably contribute to a decreased breast cancer mortality rate. With conventional mammography, Feig et al.⁵ and Anderson⁶ reported that 89% and 95%, respectively, of DCIS were observed on the basis of microcalcifications alone. Thus, to compete with conventional mammography, it is important that radiologists are able to accurately detect and diagnose microcalcifications on breast CT imaging devices.

*Address all correspondence to: Andrey Makeev, E-mail: andrei.makeev@gmail.com

A straightforward way of improving detector spatial resolution is to decrease the size of the detector pixel. However, two problems arise when designing a CZT/CdTe-based detector with very small pixels. The first is that the expense of fabricating the circuitry with small pixels becomes prohibitive, and the second is that inter-pixel charge sharing can obviate any improvement in spatial resolution. One approach to solving these problems is to estimate x-ray interaction position within the detector by evaluating local charge deposition to achieve subpixel spatial resolution on an event-by-event basis. This concept has been extensively investigated for scintillator-based nuclear medicine detectors,^{7,8} but has been studied less for photon-counting CT detectors. Ballabriga et al.^{9,10} have described the Medipix-3 inter-pixel architecture where charges are summed in 2×2 pixel clusters to improve resolution and spectroscopic performance. Ullberg et al.¹¹ have recently described a similar algorithm for a CdTe CT detector designed for counting of x-rays.

In this work, we extend our previous study¹² that described two position estimation algorithms that can be used with pixelated semiconductor detectors; maximum-likelihood (ML) estimation and a simpler and faster approach that aims to identify the quadrant of the pixel in which the x-ray interaction occurred. The latter method, which we refer to as the “quadrants” method, can be practically implemented in an application-specific integrated circuit (ASIC) without excessive limitations on the counting rate. The major change from the previously reported results is the incorporation of the effect of the fluorescent (characteristic) x-rays on the interaction position estimation. To investigate these techniques, computer simulations were performed using the COMSOL multiphysics software¹³ to model charge transport within the CZT detector, and the PENELOPE Monte Carlo (MC) tool¹⁴ to simulate nonlocal charge deposition by characteristic radiation.

2 Methods

2.1 Detector Configuration and Operating Parameters

A CZT detector was modeled as a $1 \times 1 \times 5$ mm³ rectangular volume with a continuous cathode and a 5×5 array of 160×160 μm^2 anode pixels with a pixel pitch of 200 μm [Fig. 1(a)].

Fig. 1 (a) Pixelated 5×5 anode array, (b) charge induction efficiency (CIE).

A geometry with a high detector depth to pixel size ratio emphasizes the “small pixel” effect that improves the weighting potential shape, reduces device sensitivity to hole trapping, and provides for a more uniform energy response throughout the detector volume. Only electron transport was modeled. Electron mobility was set to be $\mu_e = 850$ cm² V⁻¹ s⁻¹. A negative potential $\phi_{\text{bias}} = -600$ V was applied to the cathode, while pixelated anodes were kept grounded in the simulation. For this study, no carrier trapping was included in the transport equation.

2.2 Charge Spreading Due to Carrier Diffusion and Convection

Carrier transport in pixelated semiconductor detectors and distribution of charge pulses can be characterized by the charge induction efficiency (CIE), the ratio of the charge q_{ind} collected on a given electrode to the charge q produced by an interacting x-ray

$$\eta(\mathbf{r}, t) = q_{\text{ind}}(\mathbf{r}, t)/q. \quad (1)$$

Direct computation of η by solving the semiconductor continuity equation is challenging [especially for a densely-discretized three-dimensional (3-D) geometry], since it requires knowledge of Green’s function for all possible x-ray interaction locations in the detector volume. An effective way of calculating the induced signal by a charge produced at any location in the detector at any time was developed by Prettyman.¹⁵ Using the definition of the adjoint of a differential operator combined with the Shockley–Ramo theorem,¹⁶ and choosing the specific adjoint source term one can write the adjoint carrier continuity equation for either electrons or holes (equation for electrons is shown)

$$\frac{\partial \tilde{n}_e}{\partial t} = D_e \nabla^2 \tilde{n}_e + \mu_e \nabla \phi \nabla \tilde{n}_e - \frac{\tilde{n}_e}{\tau_e} + \mu_e \nabla \phi \nabla \psi, \quad (2)$$

where the dimensionless quantity $\tilde{n}_e$ is the adjoint electron concentration, the diffusion coefficient is defined by the Einstein relation $D_e = k_B T / q_0 \mu_e$ [cm² s⁻¹], μ_e [cm² V⁻¹ s⁻¹] is the electron mobility, ϕ [V] is the applied potential, ψ is the

dimensionless “weighting” potential for a specific electrode, and τ_e [s] is the electron trapping time. Prettyman¹⁵ demonstrated that for the appropriate initial and boundary conditions

$$\tilde{n}_e(\mathbf{r}, 0) = 0, \text{ in detector volume,} \quad (3)$$

$$\tilde{n}_e(\mathbf{r}, t) = 0, \text{ on Ohmic contact surfaces,} \quad (4)$$

$$\hat{n} \cdot \nabla \tilde{n}_e = 0, \text{ on semiconductor-insulator surfaces,} \quad (5)$$

after transforming the final-value problem to the initial-value problem by a change of variables, the solution of the adjoint Eq. (2) is equivalent to the equation which defines the CIE

$$\eta(\mathbf{r}, t) = \tilde{n}_e(\mathbf{r}, t). \quad (6)$$

Therefore, the solution of a single transient Eq. (2) gives a CIE distribution $\eta(\mathbf{r}, t)$ for an electrode of interest due to the charge produced at any location at any time. We used the COMSOL finite element method software to simulate a simple 3-D pixellated detector geometry and to solve the adjoint Eq. (2). Figure 1(b) shows a two-dimensional (2-D) slice of the CIE distribution calculated for the central pixel of the described detector model. Discrete $300 \times 300 \times 900$ CIE maps, recorded 500 ns after the creation of charge carriers, were determined for all 25 anode pixels. Such a collection of CIE maps for all detector pixels can serve as a useful measure of charge sharing between neighboring electrodes due to electron drift and diffusion.

2.3 Charge Spreading in CZT Caused by Fluorescent X-Rays

Over the clinical x-ray CT energy range (40-120 kVp), the dominant type of photon interaction in CZT is photo-electric absorption. Compton scattering accounts for only a few percent in the total interaction cross section and can be neglected. A significant fraction of incoming photons with energy above the K -edge of

Cd and Te undergoes interaction with the innermost orbital (K -shell) electron by knocking it off and exciting the atom. A smaller fraction of photons interacts with the next innermost L -shell electron. De-excitation occurs by electrons transitioning from outer to vacant inner orbits, followed by emission of fluorescent x-rays or Auger electrons. The two most prominent electron transitions in Cd and Te are K_α lines with energies $E_{K_\alpha}^{\text{Cd}} = 23.17$ keV and $E_{K_\alpha}^{\text{Te}} = 27.47$ keV.¹⁷ These characteristic x-rays are isotropically emitted and travel on average 120 and 60 μm , correspondingly, in CZT, and thus are capable of producing a sizeable charge at distances on the order of the pixel size away from the original x-ray interaction location. The two main K_α modes are accompanied by several combined electron transitions with lower energy, short-range photons. Fluorescent x-rays production can be modeled with MC electron/photon transport software. We used PENELOPE code¹⁴ to simulate a pencil beam of 50 keV x-rays incident normally on a slab of CZT. Figure 2(a) shows the spatial distribution of energy deposition for a pencil beam incident on the “top” of a CZT slab. The process is characterized by an exponential decrease in the number of interactions with depth, a symmetric distribution of deposited energy about the incident beam axis, a substantial fraction of events undergoing direct and combined fluorescent transitions, and an exponentially decaying radial spread of fluorescent energy. A vertically integrated energy distribution map is shown in Fig. 2(b).

The detector’s point-spread function for monochromatic incident radiation can be simulated by binning the MC energy deposition distribution for an x-ray pencil beam into a 3-D spatial array, normalizing it by total energy, and coupling the resulting fluorescence probability density function with the pixel induction efficiency map.

2.4 Position Determination Using Method of Maximum Likelihood

Provided that the probability density function of a random variable g , conditioned on a parameter vector θ , is represented by $f(g|\theta)$, the joint probability density of n independent, identically

Fig. 2 Energy deposited in a CZT slab by a normally incident pencil beam of 50 keV x-rays. (a) Three-dimensional (3-D) energy deposition map. Color depth indicates energy in keV. (b) Vertically integrated energy deposition map. Color scale is logarithmic.

distributed observations is given by the product of the individual densities

$$\text{pr}(\mathbf{g}|\boldsymbol{\theta}) = f(g_1, \dots, g_n|\boldsymbol{\theta}) = \prod_{i=1}^n f(g_i|\boldsymbol{\theta}). \quad (7)$$

When the conditional probability $\text{pr}(\mathbf{g}|\boldsymbol{\theta})$ is regarded as a function of the unknown set of parameters $\boldsymbol{\theta}$, for fixed data vector $\mathbf{g}$, it is called the likelihood. In an ML problem, one searches for a parameter vector $\boldsymbol{\theta}$ that will make the observed sample most probable by maximizing $\text{pr}(\mathbf{g}|\boldsymbol{\theta})$ with respect to $\boldsymbol{\theta}$. Barrett and Myers¹⁸ provide a comprehensive discussion of the ML formalism in application to position and energy determination in pixellated semiconductor x-ray detectors. In particular, they demonstrate that the likelihood for 3-D position estimation, for carrier-generation statistics with no trapping, is multivariate normal. Treating x-ray interaction position $\mathbf{r}_{\text{int}}$ as a parameter vector $\boldsymbol{\theta}$, and the set of measured pixel signals $\mathbf{N}$ as a data vector $\mathbf{g}$, the likelihood for fixed $\mathbf{r}_{\text{int}}$ can be written as

$$\begin{aligned} \text{pr}(\mathbf{N}|\mathbf{r}_{\text{int}}) &= (2\pi)^{-\frac{1}{2}M} [\det \mathbf{K}_N(\mathbf{r}_{\text{int}})]^{-\frac{1}{2}} \\ &\times \exp \left\{ -\frac{1}{2} [\mathbf{N} - \bar{\mathbf{N}}(\mathbf{r}_{\text{int}})]' \mathbf{K}_N^{-1}(\mathbf{r}_{\text{int}}) [\mathbf{N} - \bar{\mathbf{N}}(\mathbf{r}_{\text{int}})] \right\}, \end{aligned} \quad (8)$$

where the set of measured pixel signals $\mathbf{N}$ is an $M \times 1$ vector, expressed in a number of collected electrons, M is the size of the neighborhood, $\bar{\mathbf{N}}$ is the vector of expected value pixel signals, and $\mathbf{K}_N$ is the covariance matrix of the pixel array for a given $\mathbf{r}_{\text{int}}$. Barrett and Myers further show that maximizing the log-likelihood is equivalent to minimization of the quadratic form in the exponent in Eq. (8), i.e., ML position estimation is formulated as an optimization problem of finding such a parameter $\hat{\mathbf{r}}_{\text{ML}}$ that for

$$\Phi(\mathbf{N}|\mathbf{r}_{\text{int}}) = [\mathbf{N} - \bar{\mathbf{N}}(\mathbf{r}_{\text{int}})]' \mathbf{K}_N^{-1}(\mathbf{r}_{\text{int}}) [\mathbf{N} - \bar{\mathbf{N}}(\mathbf{r}_{\text{int}})], \quad (9)$$

$\hat{\mathbf{r}}_{\text{ML}} = \text{argmin} \Phi(\mathbf{r}_{\text{int}})$. We used computer modeling to simulate the expected value signal set $\bar{\mathbf{N}}$, “measured” noisy signal set $\mathbf{N}$, and pixel covariance matrix $\mathbf{K}_N^{-1}$, for the CZT detector configuration described above. Because of the presence of nonlocal charge deposition in our modeling (i.e., impinging x-ray may deposit its energy in multiple spatial locations in the detector), instead of estimating the x-ray 3-D interaction location $\mathbf{r}_{\text{int}}$, we were only concerned with its entrance coordinates $\mathbf{r}_{\text{inc}} = (x_{\text{inc}}, y_{\text{inc}})$ in a 2-D plane normal to the incidence direction. The depth of interaction z_{int} was treated as a nuisance parameter¹⁸ and was set to the mean value $\bar{z}_{\text{int}} = \mu_{\text{photo}}^{-1} \text{CZT}$, where $\mu_{\text{photo}} \text{CZT}$ is the photo-electric x-ray absorption coefficient in CZT for a given energy. Similar to a 3-D case, the 2-D ML position estimation problem was defined as the following: finding such an estimate $\hat{\mathbf{r}}_{\text{ML}}$ of $\mathbf{r}_{\text{inc}}$ that will minimize the weighted least-squares residual

$$\Phi(\mathbf{N}|\mathbf{r}_{\text{inc}}) = [\mathbf{N} - \bar{\mathbf{N}}(\mathbf{r}_{\text{inc}})]' \mathbf{K}_N^{-1}(\mathbf{r}_{\text{inc}}) [\mathbf{N} - \bar{\mathbf{N}}(\mathbf{r}_{\text{inc}})], \quad (10)$$

for a “measured” signal set $\mathbf{N}$. Simulation of the expectation value signal $\bar{\mathbf{N}}(\mathbf{r}_{\text{inc}})$ is straightforward, using the CIE matrix $\boldsymbol{\eta}(x, y, z)$ for a M pixel neighborhood, computed in COMSOL, and a fluorescent interactions probability density vector $\mathbf{p.d.f.}^{\text{fluor}}(x, y, z)$, obtained from MC. For CZT, electron-hole

pair creation energy is $\epsilon_{\text{CZT}} \approx 4.64$ eV, therefore, for monochromatic 50 keV incident photons we have

$$\bar{\mathbf{N}}(\mathbf{r}_{\text{inc}}, \bar{z}_{\text{int}}) = (50000/\epsilon_{\text{CZT}}) \boldsymbol{\eta}(\mathbf{r}_{\text{inc}}, \bar{z}_{\text{int}}) \mathbf{p.d.f.}^{\text{fluor}}(\mathbf{r}_{\text{inc}}, \bar{z}_{\text{int}}). \quad (11)$$

In order to implement the “measured” noisy signal $\mathbf{N}$, we follow the MC energy deposition history of the primary and secondary photons and introduce a sub-Poisson random deviate about a number of electrons $n_e^{(i)} = E^{(i)}/\epsilon_{\text{CZT}}$ created at each step i where energy $E^{(i)}$ was deposited, using the Fano factor¹⁹ $F \approx 0.1$ for CZT

$$n_{e \text{ sub}}^{(i)} = \text{Poisson}\{F n_e^{(i)}\} + n_e^{(i)}(1 - F). \quad (12)$$

The induced signal is obtained by multiplying $n_{e \text{ sub}}^{(i)}$ by the CIE at a current spatial location and summing over the absorbed secondary photons. Integrated circuit simulations have shown that it is reasonable to model pixel readout electronic noise for a 50 keV photon incident on a 100% efficient CZT detector as the zero-mean white Gaussian noise with root mean square (RMS) on the order of 1% at the peak voltage. Therefore, the noisy “measured” set of pixel signals can be modeled as

$$\mathbf{N} = \sum_{i=1}^{n_{\text{dep}}} n_{e \text{ sub}}^{(i)} \boldsymbol{\eta}^{(i)} + \text{Normal}\{0, \sigma_{\text{noise}}\}, \quad (13)$$

where summation is over the number of elementary energy deposition points n_{dep} for each impinging photon. In the presence of electronic noise in the pixel readout, for statistics with no carrier trapping, the conditional covariance matrix on the pixel output pulses in Eq. (10) is given by¹⁸

$$\begin{aligned} [\mathbf{K}_N(\mathbf{r}_{\text{inc}}, \bar{z}_{\text{int}})]_{mm'} &= [\bar{N}_{\text{eh}} \eta_m(\mathbf{r}_{\text{inc}}, \bar{z}_{\text{int}}) + \sigma_{\text{noise}}^2] \delta_{mm'} \\ &+ \bar{N}_{\text{eh}} (F - 1) \eta_m(\mathbf{r}_{\text{inc}}, \bar{z}_{\text{int}}) \eta_{m'}(\mathbf{r}_{\text{inc}}, \bar{z}_{\text{int}}), \end{aligned} \quad (14)$$

where $\eta_m(\mathbf{r}_{\text{inc}}, \bar{z}_{\text{int}})$ is the CIE for the m 'th pixel at a point $(\mathbf{r}_{\text{inc}}, \bar{z}_{\text{int}})$, and $\bar{N}_{\text{eh}} = \text{Var}\{N_{\text{eh}}\}/F$, with N_{eh} being the total number of electrons produced in the interaction. Electronic noise variance appears only in the diagonal elements of the covariance matrix under the assumption that channel readout noise is independent for each pixel. A nonoptimized, brute force implementation of a 2-D search was used with a $200 \times 200 \mu\text{m}^2$ area tested for each search location.

2.5 Position Determination Using “Quadrants” Method

We also investigated a simple and practical technique of subpixel position determination which does not involve the complexity and computational load of ML estimation and can be realized in the detector's readout circuitry with less penalty on the counting rate. The concept of this approach is illustrated in Fig. 3. The x-ray interaction in the center pixel of the 3×3 pixel region is indicated by the red dot. It generates a charge cloud that, by the time it reaches the anode surface, has grown to the size of the red circle. The interaction location can be narrowed down to the top left quadrant of the pixel by comparing the amount of charge detected to the left and right, as well as above and below the center pixel. The interacting (center) pixel is chosen as the one

Fig. 3 Identifying x-ray interaction position to a pixel quadrant by comparing charge pulses in a 3×3 neighborhood.

with the highest signal amplitude in the neighborhood. In the example pictured in Fig. 3, the sum signal induced on the three pixels above the hot pixel exceeds the sum signal induced on the three electrodes below it. In like manner, the total charge on the three pixels to the left of the central pixel is greater than the total charge on the three pixels to the right. If the center pixel is located at the edge of the array, the quadrant identification will instead have to be based on the charge ratio between the remaining neighbor pixel and the center pixel itself. Subdividing pixels into quadrants quadruples the effective size of the image array, i.e., localization of an x-ray interaction by the method is done using the quadrant index rather than the pixel index. Formally, the choice of the interaction quadrant can be summarized as shown in Algorithm 1 and illustrated in Fig. 4. Consider the 3×4 pixel neighborhood shown in Fig. 4. The pixels are marked off with the black lines, whereas the quadrants are marked off with

Algorithm 1 X-ray interaction pixel quadrant determination.

1: Let $a_{i,j}$ be the signal amplitude in a pixel at i -th row, j -th column in a $m \times n$ subset of pixels, $1 < i < m$, $1 < j < n$.

2: Find location (i', j') of the pixel with the maximum amplitude, $a_{\max} = a_{i',j'} = \max(a_{i,j})$, where $1 < i < m$, $1 < j < n$.

3: Compute sums of the signals in three pixels above, below, to the left and to the right of the “hot” pixel (i', j') :

$$s_{\text{abv}} = a_{i'-1,j'-1} + a_{i'-1,j'} + a_{i'-1,j'+1}$$

$$s_{\text{blw}} = a_{i'+1,j'-1} + a_{i'+1,j'} + a_{i'+1,j'+1}$$

$$s_{\text{left}} = a_{i'-1,j'-1} + a_{i',j'-1} + a_{i'+1,j'-1}$$

$$s_{\text{right}} = a_{i'-1,j'+1} + a_{i',j'+1} + a_{i'+1,j'+1}$$

4: Within a $2m \times 2n$ array of quadrants decide and return the quadrant indices of an x-ray interaction:

5: **if** $s_{\text{abv}} > s_{\text{blw}}$ **and** $s_{\text{left}} > s_{\text{right}}$ **then return** $(2i' - 1, 2j' - 1)$

6: **if** $s_{\text{abv}} > s_{\text{blw}}$ **and** $s_{\text{left}} < s_{\text{right}}$ **then return** $(2i' - 1, 2j')$

7: **if** $s_{\text{abv}} < s_{\text{blw}}$ **and** $s_{\text{left}} > s_{\text{right}}$ **then return** $(2i', 2j' - 1)$

8: **if** $s_{\text{abv}} < s_{\text{blw}}$ **and** $s_{\text{left}} < s_{\text{right}}$ **then return** $(2i', 2j')$

		j							
		1	2	3	4	5	6	7	8
i	1	1,1	1,2	1,3	1,4	1,5	1,6	1,7	1,8
	2	2,1	2,2	2,3	2,4	2,5	2,6	2,7	2,8
	3	3,1	3,2	3,3	3,4	3,5	3,6	3,7	3,8
	4	4,1	4,2	4,3	4,4	4,5	4,6	4,7	4,8
	5	5,1	5,2	5,3	5,4	5,5	5,6	5,7	5,8
	6	6,1	6,2	6,3	6,4	6,5	6,6	6,7	6,8

Fig. 4 Pixel and quadrant array indices.

the red lines. If the highest amplitude was recorded, for instance, in the pixel $(i = 2, j = 3)$, the method will decide which quadrant of this pixel to assign the interaction location based on the sums of the signals from the three pixels immediately above, below, to the left, and to the right of the center one. For example, if the sum of the signals from pixels $(1,2)$, $(1,3)$, $(1,4)$ exceeds the sum of the signals from pixels $(3,2)$, $(3,3)$, $(3,4)$ and the sum of the signals from pixels $(1,2)$, $(2,2)$, $(3,2)$ exceeds the sum of the signals from pixels $(1,4)$, $(2,4)$, $(3,4)$, then the x-ray interaction will be localized to the upper-left quadrant of the pixel $(2,3)$. From line 5 of the pseudocode Algorithm 1, the x-ray interaction coordinates on a $2m \times 2n$ quadrant grid will then be $(2 \times 2 - 1, 2 \times 3 - 1) = (3,5)$.

2.6 Pixel Region-of-Interest and Electronic Noise Amplitude

To study the algorithm performance in estimating the position of x-ray incidence on the detector, we simulated 2000 events at each point in the square region $300 \leq x \leq 700 \mu\text{m}$, $300 \leq y \leq 700 \mu\text{m}$ of the modeled detector, as shown in Fig. 5. Such a selection embraces a spatial region sufficient to capture the

Fig. 5 Selected area used for position estimation.

key areas (the pixel surface and the inter-pixel boundaries) of the recurring pattern of the error distribution, without redundant coverage. Based on simulations of a new four-sided abutable ASIC being developed for breast CT,²⁰ two levels of electronic noise were modeled, 1% (nominally expected) and 2.5% (upper margin) RMS amplitude at the peak voltage.

3 Results

3.1 Position Accuracy for Method of Maximum Likelihood

An RMS error between the ML-estimated and true interaction position was used as a measure of position uncertainty

$$\sigma_u = \left[\frac{1}{N_{\text{evt}}} \sum_{i=1}^{N_{\text{evt}}} (u_i - u_{\text{true}})^2 \right]^{1/2}, \quad (15)$$

where u stands for either x or y . Contour plots in Fig. 6 show RMS errors on x - and y -coordinates of x -ray interactions, as well as the total RMS error $\sigma_{\text{tot}} = (\sigma_x^2 + \sigma_y^2)^{1/2}$ for the ML method, calculated over the selected region for an electronic noise RMS amplitude of 1%. The ML algorithm achieves its lowest position estimation uncertainty $\sigma_{x,y}^{\text{ML}} \approx 14 \mu\text{m}$ in the inter-pixel gap regions ($x, y = 400 \mu\text{m}$; $x, y = 600 \mu\text{m}$), where the charge sharing is the most significant and the method can effectively utilize information from multiple pixels. The highest estimation uncertainty of $\sigma_{x,y}^{\text{ML}} \approx 40 \mu\text{m}$ is observed in the regions along the pixel center lines ($x, y = 300 \mu\text{m}$; $x, y = 500 \mu\text{m}$; $x, y = 700 \mu\text{m}$), where the charge sharing between the electrodes is minimal and the charge induced by an x -ray interaction is mostly localized to a single pixel. It is also interesting to notice that the ML algorithm demonstrates the best performance in the areas where the charge sharing is highest between the pixels along the measured coordinate axis and lowest between the pixels in the transverse direction, such that the shared charge is maximally used by the relevant electrodes. Likewise, the ML performance is the poorest in the areas where the charge sharing is minimal between the pixels in the direction of interest and highest between the electrodes along the transverse axis. This explains the presence of “cold” (deep blue) and “hot” (deep red) clusters in the contour plots of Figs. 6(a) and 6(b). The total RMS position error σ_{tot} , presented in Fig. 6(c), varies from approximately $22 \mu\text{m}$ in the inter-pixel gaps centers to

about $56 \mu\text{m}$ in the pixel centers. Averaged over the sampled area $300 \leq x, y \leq 700 \mu\text{m}$, values of RMS position errors are, respectively, $\bar{\sigma}_{x,y}^{\text{ML}} \approx 27 \mu\text{m}$ and $\bar{\sigma}_{\text{tot}}^{\text{ML}} \approx 40 \mu\text{m}$. For a simulated detector geometry with the reported operating parameters, the ML method provides for an accurate subpixel position estimator with the mean x and y RMS errors on the order of one-seventh of the pixel pitch and a mean total RMS position uncertainty on the order of one-fifth of the pixel pitch. The ML method is an efficient statistical estimator that asymptotically approaches the Cramér–Rao lower bound on the parameter variance, i.e., it approaches the best achievable position measurement performance among the statistical algorithms. The main concern with the use of the ML algorithm in real detectors is its speed performance on an actual readout ASIC, which could impose a limitation on the detector counting rate in applications with high x -ray flux.

3.2 Position Accuracy for “Quadrants” Method

The results of RMS position error measurements for the “quadrants” method are summarized in Fig. 7. Due to the sampling, snap-to-grid-like nature of the algorithm, the position variance is highest between the quadrant centers and lowest at the quadrant center locations. Unlike the method of ML, the “quadrants” method struggles the most at the centers of the inter-pixel gaps where identification of the interaction pixel is least reliable. Averaged over the sampled area, the RMS position errors are $\bar{\sigma}_{x,y}^{\text{quad}} \approx 50 \mu\text{m}$ and $\bar{\sigma}_{\text{tot}}^{\text{quad}} \approx 70 \mu\text{m}$. As expected, ML produces notably more accurate results. Nevertheless, taking into account the simplicity of the “quadrants” algorithm and its potential computational advantage over ML estimation, it is still capable of attaining a position measuring uncertainty on the order of a quarter of a pixel pitch for the simulated detector geometry and operating parameters.

3.3 Maximum Likelihood Versus “Quadrants” Performance for Different Levels of Electronic Noise

Shown in Fig. 8 is the descriptive comparison of the total RMS position variance profiles across the representative lines for the ML and the “quadrants” methods for pixel noise RMS amplitude of 1% and 2.5%. The profile at $y = 500 \mu\text{m}$ passes through the center of the pixel. The profile at $y = 600 \mu\text{m}$ passes through the center of the inter-pixel gap. Here, it is clearly

Fig. 6 Maximum likelihood (ML): position measurement uncertainty for noise RMS amplitude 1%. Thin lines at $x, y = 400, 600 \mu\text{m}$ indicate pixel boundaries. (a) x -position root-mean-square (RMS) error; $\bar{\sigma}_x^{\text{ML}} \approx 27 \mu\text{m}$, (b) y -position RMS error; $\bar{\sigma}_y^{\text{ML}} \approx 27 \mu\text{m}$, (c) total RMS error; $\bar{\sigma}_{\text{tot}}^{\text{ML}} \approx 39 \mu\text{m}$.

Fig. 7 “Quadrants” method: position measurement uncertainty for noise RMS amplitude 1%. Thin lines at $x, y = 400, 600 \mu\text{m}$ indicate pixel boundaries. (a) x -position RMS error; $\sigma_x^{\text{quad}} \approx 48 \mu\text{m}$, (b) y -position RMS error; $\sigma_y^{\text{quad}} \approx 48 \mu\text{m}$, (c) total RMS error; $\sigma_{\text{ML}}^{\text{quad}} \approx 68 \mu\text{m}$.

Fig. 8 Total RMS position error profile plots through the center of the pixel ($y = 500 \mu\text{m}$) and through the center of the inter-pixel gap ($y = 600 \mu\text{m}$) for the ML and “quadrants” methods.

observed that the ML estimation performs worst for x-rays interacting at the center of pixels, whereas the quadrants method performs worst for x-rays interacting at the edge of pixels. The ML also provides more a uniform resolution performance throughout the chosen segments than the “quadrants” algorithm. It is interesting to notice that the increase of pixel RMS noise from a nominal anticipated amplitude of 1% to a higher value of 2.5% only has a marginal effect on the position uncertainty for both ML and “quadrants” algorithms. We link this insensitivity to electronic noise with the fact that at these magnitudes, its impact on position estimation is weak compared to the uncertainties in measured pixel signals introduced by characteristic radiation in CZT.

3.4 Probability of Correct Localization of Interaction Pixel/Quadrant

The presence of stochastic noise in the pixel readout, fluorescent x-rays, and charge spreading can result in erroneous identification of the interaction pixel and the quadrant. These factors will degrade the efficiency of localization of the x-ray interaction

Fig. 9 Pixel quadrant Q3 is illuminated to measure the probability of correct localization.

coordinates and decrease the accuracy of the “quadrants” method. In the model, the probability of correct localization (PCL) of a pixel or a quadrant can be estimated by calculating the fraction of events in which the pixel/quadrant is correctly identified at each point within it. This is illustrated in Fig. 9, where the shaded area is finely sampled with the same number of incident x-rays simulated at each point. Contour plots in Fig. 10 show the probability of correct localization maps for a given pixel and its quadrants for electronic noise RMS amplitudes of 1% and 2.5%. The contour area corresponds to the area of the pixel in μm^2 . The plots in the left column represent the PCL for a pixel, whereas the plots in the right column represent the PCL for the four quadrants of a pixel combined. The first observation made from these maps is that the amplitude of electronic noise does not have a significant impact on the region of reliable pixel/quadrant identification, leading only to a slight reduction of the “good” area with the electronic noise amplitude changing from 1% to 2.5% RMS. The probability of misidentifying the interaction (hot) pixel increases toward its boundaries. Similarly, for the quadrants, the PCL deteriorates closer to their boundaries, experiencing a more significant drop near the center of the pixel where the charge sharing is minimal, leading to smaller and closer in magnitude signals induced in the neighboring pixels, used for making decisions about interaction localization. It is instructive to look at how the presence of K -escape x-rays influences the “quadrants” method efficiency. One can simply “turn off” modeling of the fluorescent photon

Fig. 10 Probability of correct identification of the interacting pixel (left column) and its quadrants (right column) when the fluorescent interactions are modeled. Color contour represents a $200 \times 200 \mu\text{m}^2$ area of the central pixel in the 5×5 anode array. (a) Electronic noise RMS 1%, (b) electronic noise RMS 1%, (c) electronic noise RMS 2.5%, (d) electronic noise RMS 2.5%.

production in the PENELOPE photon transport configuration, such that the entire incident x-ray energy is locally deposited.

The effects of charge sharing due to carrier diffusion and electronic noise are still present. The PCL contour plots analogous to the ones in Fig. 10, but with fluorescence processes excluded, are shown in Fig. 11. It is easy to observe from comparison of (the left columns of) Figs. 10 and 11 that the interaction pixel misidentification is primarily caused by escaping K x-rays. Correct quadrant localization is also worsened by the presence of the characteristic radiation. Analysis of the two types of PCL maps also indicates that the effect of electronic noise on the quadrant recognition is more prominent in the absence of the fluorescent photons.

3.5 Maximum Likelihood and “Quadrants” Methods Compared for Visualizing Microcalcifications

Both position estimation methods considered here lead to a space-variant resolution effect. To illustrate how the resolution nonuniformity affects the visual appearance of the projection image, a $330 \mu\text{m}$ diameter microcalcification sphere was simulated and its projections were obtained using ML and “quadrants” algorithms. In this example, the microcalcification was placed in the center of the $400 \times 400 \mu\text{m}^2$ area used for error characterization, as described above. No biological background surrounding the calcification was simulated. Figure 12 shows the “true” and the algorithm-produced projection images. The

grayscale in the images corresponds to a value of the line integral $\ln(I/I_0)$ in a pixel, as defined by the Beer–Lambert law. As expected, the ML projection better resembles the size and the shape of the original sphere and also achieves a higher contrast as compared to projection produced by the “quadrants” method. The profiles drawn through the center of the projection images are presented in Fig. 13. The ML estimate closely follows the true profile at the center region of the sphere, but starts deviating from it toward the boundaries, while the “quadrants” method consistently underestimates the line integral values in the center and does not quite reach zero in the background. This decreases the dynamic range of the image and results in a less well-defined edge. Nonetheless, the inferior RMS error of the “quadrants” method does not result in dramatic image quality degradation. Taking into consideration its simplicity and lower computational load, the method can still produce useable results, with its applicability depending on a particular detection task. Here, we only provide a subjective comparison based on visual appearance of the projections of the object. In the future, the assessment of the detection performance should be conducted with objective measures such as receiver operating characteristic analysis.

4 Discussion

We examined the possibility of achieving subpixel position resolution with a CZT semiconductor detector by evaluating the charge sharing distribution over a pixel region of interest. A

Fig. 11 Probability of correct identification of the interacting pixel (left column) and its quadrants (right column) when the fluorescent interactions are not modeled. Color contour represents a $200 \times 200 \mu\text{m}^2$ area of the central pixel in the 5×5 anode array. (a) Electronic noise RMS 1%, (b) electronic noise RMS 1%, (c) electronic noise RMS 2.5%, (d) electronic noise RMS 2.5%.

simple pixellated detector geometry was modeled and uniformly illuminated by a monoenergetic 50 keV x-ray beam and the spatial resolution in 2-D was analyzed for the two position estimation algorithms: the method of ML and the “quadrants” method.

Our originally reported results¹² did not account for an important mechanism of nonlocal charge deposition—fluorescent (characteristic) radiation in CZT for incident photons with energy exceeding the *K*-edge of Cd and Te. Here, we include the simulation of the secondary *K*-escape photons in CZT which,

due to their relatively long mean free path, contribute noticeably to the charge spreading over the small anode pixels.

The focus of this work was to investigate improvements in spatial resolution resulting from implementing position estimation algorithms using local charge deposition. Another possible limitation with these detectors is spectral distortion, and thus a logical extension to the proposed algorithms would be to also estimate photon energy. Ullberg et al.¹¹ have described a charge sharing correction algorithm implemented on a CdTe detector with $100 \mu\text{m}$ pixels. This algorithm estimates energy from the local charge deposition, and thus greatly improves energy

Fig. 12 Projection of a simulated $d = 330 \mu\text{m}$ microcalcification (hydroxyapatite sphere) for electronic noise RMS amplitude of 1%. Grayscale represents the value of $\ln(I/I_0)$ in a pixel. (a) True projection of a sphere, (b) projection using ML method, (c) projection using “quadrants” method.

Fig. 13 Projection profiles through the center of the sphere for the two methods.

resolution and spectral distortion. Ballabriga et al.^{9,10} have described the Medipix-3 chip that also minimizes spectral distortion by using a scheme where neighboring pixels communicate with each other.

The ML estimation method requires an accurate model of the likelihood function. This function can be modeled using either simulations, as described here, or by using experimental measurements, for example by generating a narrow beam incident on the detector at many locations over the pixel. Errors in modeling the likelihood function will cause additional bias in the estimate. A full analysis of how these modeling errors would propagate into the estimation accuracy is beyond the scope of this study, but should be evaluated in future studies.

Our nonoptimized, brute force search over ML parameter space, implemented in sequential CPU code, was approximately 20 times slower compared to the “quadrants” method. This number, however, should not be regarded as a performance measure of the method realized on the actual hardware. Hesterman et al.²¹ examined the ML position estimation algorithm to obtain interaction locations in compact gamma cameras. Their optimized contracting-grid search method for ML-estimation problems in multidimensional spaces was implemented on a field-programmable gate array, PlayStation 3 Cell/BE processor, and a graphics processing unit (GPU) supercomputer. For a 2-D search on the Cell/BE processor, the reported speed gain was a factor of 20× compared to a regular CPU computation, while the GPU implementation of a 3-D search showed a remarkable 250× speed increase.

5 Conclusions

The ML method, as an efficient statistical estimator that asymptotically achieves the Cramer–Rao bound, exhibits good spatial resolution. Specifically, for a simulated CZT detector, with a 200 μm pixel pitch and an anticipated level of pixel readout RMS noise of 1%, it results in position uncertainty for x - and y -coordinates of x -ray interactions ranging in $14 \lesssim \sigma_{x,y}^{\text{ML}} \lesssim 40 \mu\text{m}$, depending on the interaction location. This result is rather different from our previous finding¹² $2 \lesssim \sigma_{x,y}^{\text{ML,no fluor}} \lesssim 15 \mu\text{m}$, which did not account for characteristic photons, and confirms that the presence of fluorescent x -rays has a substantial detrimental effect on spatial resolution. The “quadrants” method is computationally inexpensive and can be realized in the detector’s ASIC with a rather moderate reduction of the counting rate.¹¹ Our

modeling shows that RMS error on x -ray interaction position for the “quadrants” method varies within $27 \lesssim \sigma_{x,y}^{\text{quad}} \lesssim 70 \mu\text{m}$ for the same RMS noise amplitude of 1% and the same detector geometry. As in a case with ML, these resolution values exhibit a departure from our earlier submitted result,¹² $2 \lesssim \sigma_{x,y}^{\text{quad,no fluor}} \lesssim 50 \mu\text{m}$, without characteristic x -ray production included in the model. Both position estimation algorithms show little sensitivity to electronic noise. We explain this by the fact that for anticipated noise levels $1\% \leq \sigma_{\text{noise}}/V_{\text{peak}} \leq 2.5\%$, where V_{peak} is the peak voltage of the signal pulse in the pixel, its effect on position estimation is relatively weak compared with the variations in measured pixel signals induced by characteristic x -rays in CZT.

We modeled how the space-variant resolution effect for the two methods will manifest itself in the image projections for a $d = 330 \mu\text{m}$ microcalcification sphere. The ML-produced image has high contrast and exhibits good resemblance to the projected object, with microcalcification’s shape and size close to the true values. The projection image, obtained using a much more simple “quadrants” method, has lower contrast and more distortions to the sphere’s shape and size. Nonetheless, due to its simplicity and speed, it can still produce useful subpixel resolution projections for certain detection tasks.

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Andrey Makeev is a senior staff fellow at the Center for Devices and Radiological Health (CDRH), United States Food and Drug Administration (FDA). He earned his PhD in computational sciences & informatics from George Mason University in 2010. His current

research is focused on photon-counting detectors for breast imaging, iterative reconstruction algorithms, and computer modeling of CT systems.

Martin Clajus received his doctorate in physics from ETH Zurich in 1991. He is currently vice president of technology at NOVA R&D. His research interests are in the development of innovative x-ray imaging systems for defense and medical applications.

Scott Snyder received his BS degrees in mathematics and physics from California Polytechnic University at San Luis Obispo in 1984. He is currently vice president of operations at NOVA R&D, Inc. His research interests are in x-ray instrumentation for medical and defense applications.

Xiaolang Wang received her PhD in electrical and computer engineering from John Hopkins University in 2011. Her research interests are focused on developing methods for improving the performance of CT systems by incorporating novel semiconductor photon counting x-ray detectors.

Stephen J. Glick received his PhD in biomedical engineering from Worcester Polytechnic Institute in 1991. He is currently a senior staff fellow at the Center for Devices and Radiological Health (CDRH), United States Food and Drug Administration (FDA). His research interests are focused on several aspects of breast tomosynthesis and breast CT, including radiation dose, imaging technique optimization, evaluation of iterative reconstruction methods, detection studies for lesions and microcalcifications, and aspects of photon counting detectors for CT.