Monte Carlo Investigation of the Charge Sharing Effects in 3-D Position Sensitive CdZnTe Gamma Ray Spectrometers

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Abstract

Charge sharing effects in a 3-D position sensitive CdZnTe detector have been investigated by Monte Carlo simulations and experimental measurements. The charge sharing is mainly caused by the range of electrons, x-ray emission following by photoelectric interactions, and the diffusion of charge carrier electrons during their drift towards the anodes. A simple model has been developed to include the diffusion effect in the Monte Carlo simulation. Good agreement has been achieved for various irradiation and bias conditions. Based on our model simulations, a 1 mm optimal pixel size is recommended for future 1 cm thick CZT detectors for 662 keV gamma rays.

I. INTRODUCTION

Due to their large band gaps and high atomic numbers, compound semiconductor materials such as HgI, CdTe and CdZnTe are attractive as room temperature radiation detectors. But with their severe charge carrier trapping and low hole mobility, conventional planar detectors made from these materials have poor spectroscopic performance. The single carrier technique, using coplanar anodes[1, 2] or pixelated anode geometry [3], can eliminate most of the energy resolution degradation associated with poor hole transport. For our 3-D position sensitive detectors [4], the 3-D position sensitivity not only provides imaging capability, but also permits pulse amplitude correction for the electron trapping and material non-uniformity in the crystal. While an energy resolution of 1.7% FWHM has been observed at 662 keV for single pixel events from the entire volume of these $1cm^3$ cubic detectors, the energy resolution of multi-pixel events is significantly worse than that predicted by summing up the signals from individual pixels. This degradation is mainly caused by the timing uncertainty associated with the sample and hold circuitry used to capture pulse amplitudes [4]. While this sample and hold problem should be eliminated with a new design readout chip, the energy resolution from multi-pixel events will still be much worse than that for single pixel events. This is because of the quadratic summation of the electronic noise from multiple channels and any incomplete charge collection due to finite threshold for individual pixels. In this respect, for better spectroscopic performance, using larger pixel dimensions would reduce the fraction of multi-pixel events. On the other hand, smaller pixels enhance the small pixel effect and offer higher position resolution, which is better for individual voxel non-uniformity corrections and for imaging purposes. In order to improve the design of future devices, it is critical to understand the factors that contribute to the charge sharing between neighboring pixels.

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To identify the factors which contribute to charge sharing, we first analyze the measurement multi-pixel fractions using Monte Carlo simulations under various conditions. A simple model based on EGS4 is then developed to investigate the charge sharing effects for our 3-D CdZnTe detectors. Finally, charge sharing effects at various pixel sizes are simulated using our model,and will yield an optimal pixel size for 662 keV gamma rays.

II. CHARGE SHARING EFFECT

The energy spectra from 662 keV gamma rays incident from the detector's cathode side were sorted by the number of anode pixels yielding signals for each measured event . The fraction of full energy peak events as a function of pixel number was obtained for the entire crystal and the results are shown in Figure 1. Results from Monte Carlo simulations using EGS4,

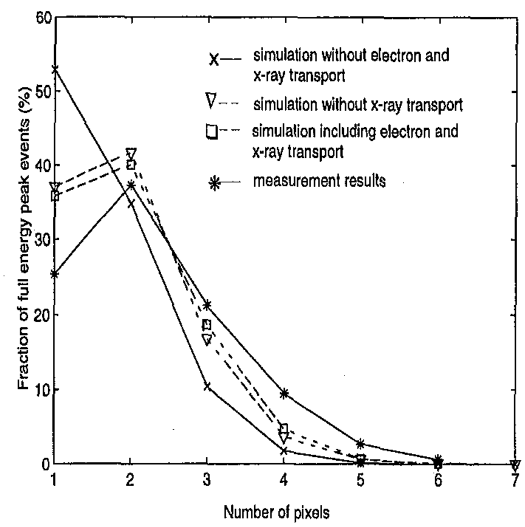

Figure 1: Measured and simple Monte Carlo simulated multi-pixel event fractions

which ignore electron and x-ray transport, are also shown in Figure 1. The simple Monte Carlo simulations predict that more than 50% of 662 keV gamma ray full energy deposition events correspond to single pixel events, and drops quickly to 2% for a pixel multiplicity of four. Our measurements show that only 25% of full energy events are single pixel events, and the fractions of multi-pixel events are much higher than that predicted by these simulations. This suggests significant charge sharing between neighboring pixels.

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There are several factors that can contribute to the charge sharing effect. These include the range of electrons (photoelectrons and Compton scatter electrons), transport of K x-rays following photoelectric interactions, and the diffusion of the charge carrier electrons during their drift towards the anode. The simulated electron cloud lateral extension (defined as maximum lateral distance for each event) distribution for photoelectric interactions at several gamma-ray energies are shown in Figure 2. At 662 keV, this distribution centers around

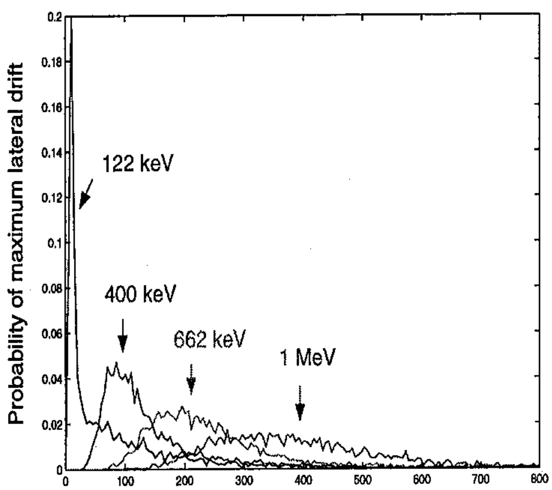

Figure 2: Simulated electron cloud lateral extension distribution

0.2 mm. The mean free path of Cd or Te K x-ray in CdZnTe is ~0.1mm [5]. Note that both of these are the same magnitude as the 0.7*0.7 mm pixel size. As shown in Figure 1, when electron and x-ray transport are included in the Monte Carlo simulation, the single-pixel fraction decreases to 35%. This indicates that nearly one-third of the single interaction events have charge sharing between neighboring pixels due to electron and x-ray transport. From our CdZnTe measurements[6], the electron mobility is around 1000 $cm^2/(V\text{-}s)$. From the Einstein relation, this gives a diffusion coefficient D= 26 cm^2/s. For our detectors with a drift time of 500 ns, this implies a diffusion length of $L=\sqrt{2Dt} = 50\mu m$. L therefore can not be neglected with only a 0.7 mm pixel dimension, and the diffusion contributions to charge sharing can not be ignored. As shown in Figure 1, even after including electron and x-ray transport in the simulation, the measured single pixel fraction is still 10% lower than predicted by simulation. In order to correctly simulate charge sharing in our pixelated detector, charge carrier diffusion must also be included.

III. A Simple Model for Charge Carrier Diffusion

Following the generation of electrons and holes from the incident radiation, when detrapping is neglected, charge carrier movement is governed by the general time-dependent Boltzmann transport equation [7]:

$$\frac{\partial n}{\partial t} = [\nabla \bullet (\mu \nabla \varphi) + \nabla \bullet (D \nabla) - \frac{1}{\tau}] \bullet n \quad (1)$$

where n is the charge carrier density, φ is operating potential, τ is charge carrier lifetime,μ is mobility, and D is the diffusion coefficient.

Since the pixel dimension is much smaller than the detector thickness, and the bias voltage between the anode pixels and the guard grid is much smaller than the bias voltage between the cathode and the anodes, the electric field is uniform in most of the volume of the detector (except very near the anode surface) [8]. Under this uniform electric field approximation, Eq.(1) can be written as:

$$\frac{\partial n}{\partial t} = \mu E \frac{\partial n}{\partial z} + D(\frac{\partial^2 n}{\partial x^2} + \frac{\partial^2 n}{\partial y^2} + \frac{\partial^2 n}{\partial z^2}) - \frac{n}{\tau} \quad (2)$$

where E=V/d is the electric field along the z (depth) direction in the detector,V is the bias voltage between cathode and anodes surface,d is the detector thickness.

With the initial condition n=$\delta(r)$, one can obtain the impulse response function from Eq.(2) as:

$$n = \frac{exp(-t/\tau)}{\sqrt{(4\pi Dt)^3}} exp(-\frac{x^2 + y^2 + (z - \mu Et)^2}{4Dt}) \quad (3)$$

Eq.(3) is a Gaussian distribution which decays exponentially with time and has the distribution center moving at the drift velocity μE. Since the diffusion contribution to charge sharing is only related to the electrons' lateral spread, one can neglect the diffusion along the transport direction z and obtain a depth dependent lateral spread function by integrating Eq.(3):

$$f(z) = \frac{1}{4\pi DT_d} exp(-\frac{x^2 + y^2}{4DT_d}) \quad (4)$$

where $T_d = z/\mu E$ is the drift time, and z is the distance from the collecting anode surface.

Since the interaction among charge carrier electrons can be neglected, the lateral spread function Eq.(4) could be ideally applied to each point along the electron trajectories simulated by EGS4. But in order to reasonably simulate electron transport in the crystal, the electron energy loss at each step can be only a few percent of its energy. Since there are ~1000 steps to simulate the trajectory of a 662 keV gamma ray photoelectron,applying Eq.(4) at each step would be computationally prohibitive.

In order to reduce the simulation time, we discretized the detector depth into 200 bins and performed a prior calculation of the lateral spread functions f(z_i). During the simulation, the proper spread functions can then be applied directly. Further, note that the Gaussian spread function in Eq.(4) has 99% of the distribution concentrated between $\pm 3\sqrt{2DT_d}$. The lateral spread is only important when the shortest distance between the energy deposition location and the nearest pixel boundary is smaller than $3\sqrt{2DT_d}$. The detector volume can be regarded as two regions: a charge sharing region ($\pm 3\sqrt{2DT_d}$ around pixel boundaries) and a non-sharing region. One needs only to apply lateral spread function in the charge-sharing region. Furthermore, we divided the energy loss trajectories in the charge-sharing region into 10μm segments, and applied the pre-caculated lateral spread function to these segments instead of to each point.

Using this approach, the additional computation time is only about 10% larger than a normal EGS4 simulation. Figure 3 shows excellent agreement between the simulated

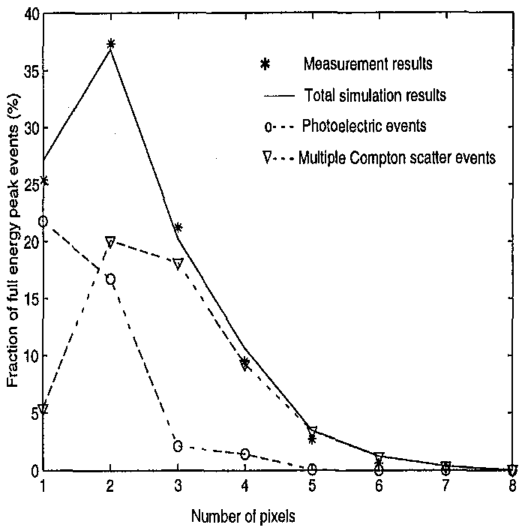

Figure 3: Multi-pixel events fractions for 662 keV gamma ray incident from cathode side(including diffusion in the simulation)

and measured charge sharing results at 662 keV. In order to estimate the contribution from diffusion and to further test our model, the charge sharing at 122 keV was measured and simulated under two irradiation conditions (on the anode side and cathode side) and two bias voltages (1400 V and 2000 V). For 122 keV gamma rays,the photoelectric effect dominates the gamma ray interactions in CdZnTe, and most interactions occur near the incident side. When the gamma rays are incident on the anode surface, charge carrier electrons drift only a short distance before they are collected by the anodes. Diffusion should not contribution to charge sharing, independent of the bias voltage. This can be seen in Figure 4 from similar single pixel events fractions. The measurements and simulations in Figure 4 agree very well. When gamma rays are incident on the cathode side, most charge carrier electrons will have to drift the full detector thickness to be collected. At the lower bias, there should be more contribution from diffusion to charge sharing. As shown in Figure 5, the single pixel event fraction at 1400 V is about 10% lower than that at 2000 V. Again, the measurements and the simulations agree very well, indicating our simple model for diffusion is adequate to simulate charge sharing effects.

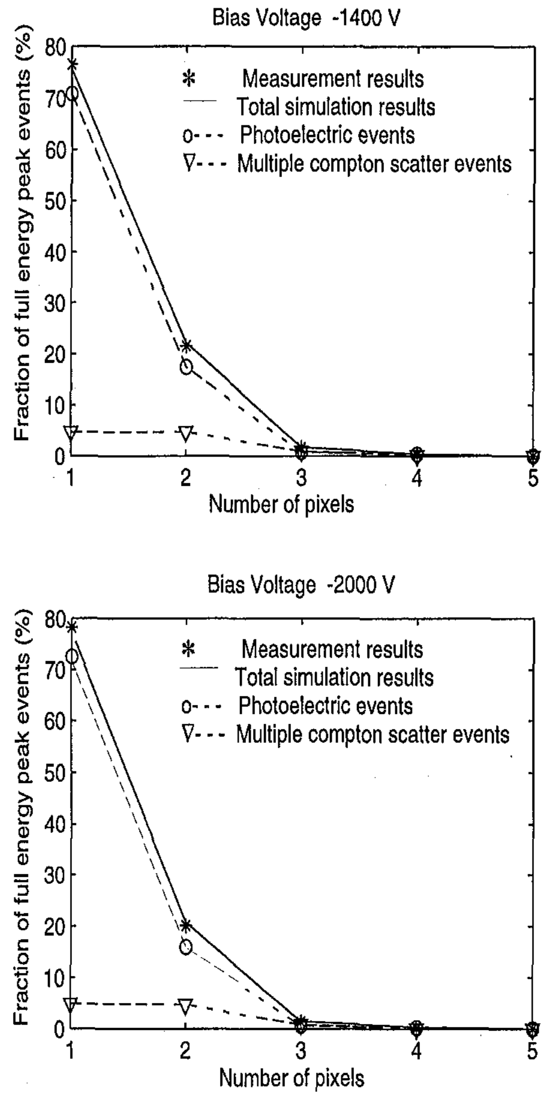

Figure 4: Multi-pixel events fractions for 122 keV gamma rays incident from anode side for 1400V (top) and 2000V (bottom)

IV. Optimization of the Pixel Dimension

In order to obtain better spectroscopic performance of the detector, larger pixel dimensions are desired to reduce the fraction of multi-pixel events. On the other hand, smaller pixels are better for single-polarity charge sensing and provide higher position resolution for imaging and non-uniform charge transport corrections in the material. Figure 6 shows the calculated charge sharing at 662 keV incident energy for various pixel sizes. As the pixel size increases from 0.5 mm to 1.5 mm, the probability of a single interaction event being recorded as multi-pixel event due to charge sharing dramatically decreases from 45% to 17%. On the other hand, the probability of multiple interactions being recorded as single pixel events slowly increases from 11% to 24%. For Compton imaging purposes, if one wants to independently record each gamma ray interaction in the detector, a pixel dimension of $\sim$ 1.1 mm should be chosen. For better spectroscopic performance, $\sim$1 mm pixel dimension should be chosen

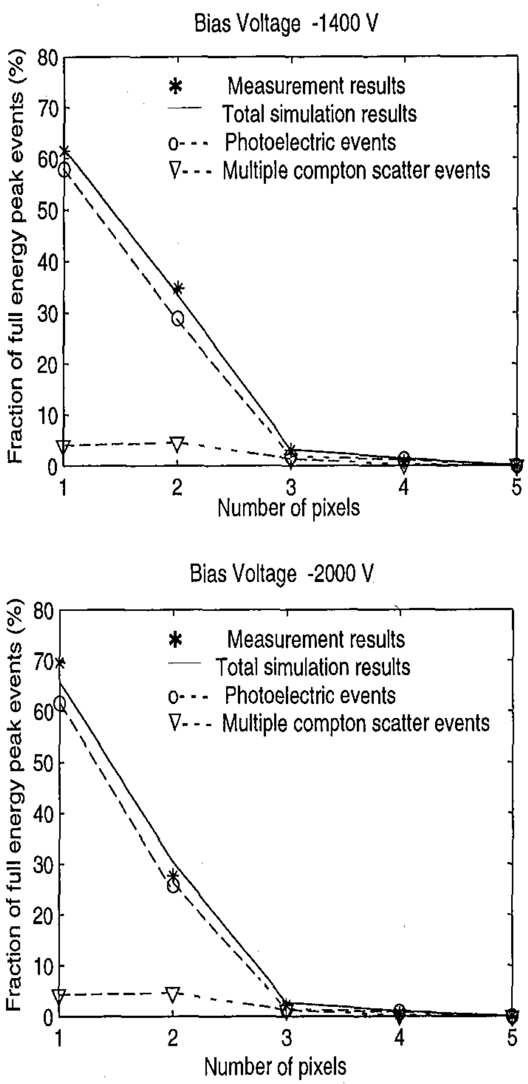

Figure 5: Multi-pixel events fractions for 122 keV gamma rays incident from cathode side for 1400V (top) and 2000V (bottom)

considering the rapid and slow decrease before and after that region for the probability of charge sharing.

V. CONCLUSION

Combining Monte Carlo simulations and experimental data, the charge sharing effect in our 3-D position-sensitive detector has been investigated. We found that the charge sharing can be accounted for by electron transport, x-ray emission following by photoelectron generation, and the diffusion of the electrons during their drift towards the anode. A simple model which included the diffusion effect significantly improved accuracy of the Monte Carlo simulations. Excellent agreement was achieved between simulations and measurements of the fractions of multi-pixel events. In order to improve future detector designs, Monte Carlo simulations were performed to investigate the charge sharing effect at different pixel dimensions for 662 keV gamma rays on 1 cm thick detectors. An optimum pixel size of about 1 mm is indicated.

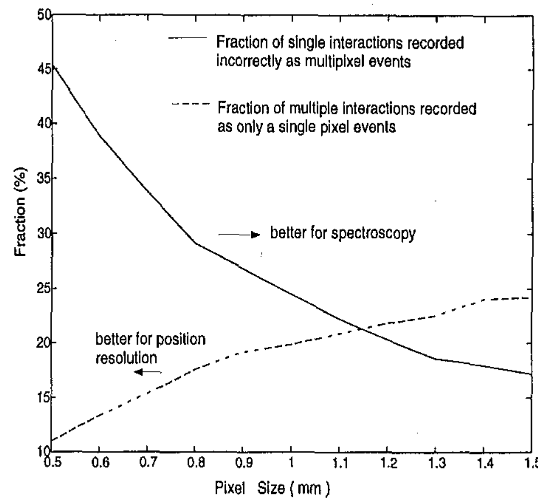

Figure 6: Charge sharing fraction vs. pixel size for 662 keV gamma rays at 2000V bias voltage

VI. ACKNOWLEDGEMENTS

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VII. REFERENCES

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