Numerical Modelling of Charge-Sharing in CdZnTe Pixel Detectors

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Abstract

In this paper, we describe our study of charge-sharing events in CdZnTe detectors being developed for the HEFT telescope. We specify the detector design, and discuss an experiment we have performed to investigate charge sharing between pixels. We have also developed a numerical model to study the charge transport in the detector. It emulates the physical processes of charge transport within the CdZnTe crystal, especially the process of drift. We discuss this numerical model of the detector in detail here. With our numerical model, we are able to reproduce the general features of the charge-sharing events. We have found that the amount of charge loss is very sensitive to the surface $\mu t$, the product of charge mobility and trapping time, of CdZnTe; here, we present estimates of $(\mu t)_{\text{surface}}$ from our model. Further work will focus on more detailed analysis of diffusion, in order to gain a complete understanding of these charge-sharing events in CdZnTe pixel detectors.

I. INTRODUCTION

Our group at the California Institute of Technology have been developing CdZnTe pixel detectors for use in astrophysical applications, and specifically, the High Energy Focusing Telescope (HEFT) \cite{1}. These detectors operate at hard X-ray energies, from 5 keV to 150 keV. Our goal is to achieve the highest spectral resolution possible with our detectors by having a custom-designed, low-noise VLSI readout circuit, by optimizing the pixel contact geometry, and by careful processing of the pulse height data.

In our earlier papers \cite{2}, we have reported studies of our detector performance for single-pixel events—events in which incident photons are absorbed by photoelectric effect within a single pixel, with all the induced charges collected by the pixel. This paper describes our subsequent effort in studying charge-sharing events—events in which photons are absorbed between two pixels, inducing charges that are shared between the pixels. Our experiments for testing the detectors have been described in Bolotnikov et al \cite{3}. We shall first summarize the experiments, and then describe a numerical model we have developed in an attempt to understand and interpret the experimental results.

II. DETECTOR GEOMETRY

Our prototype CdZnTe detector geometry is an array of 8 x 8 pixels. The pixel pitch has dimensions 680 $\mu$m x 650 $\mu$m (centre-to-centre spacing), and the CdZnTe crystal is 2 mm thick between the cathode and anode planes. The cathode plane is covered entirely with a single platinum contact, set at the negative bias voltage; the geometric configuration of the anode plane is shown in Figure 1. At the centre of each pixel is a rectangular metal contact for the anode, set at ground potential.

![Figure 1: Anode-plane configuration of our CdZnTe detector. Drawn to scale.](image)

At the perimeter, the pixel contact is surrounded by a 'steering electrode', set at a negative potential relative to ground at the anode. The steering electrodes of all pixels are connected into a grid, as shown in Figure 1. Between the anode contacts and the grid of steering electrodes are bare surfaces of CdZnTe, which we refer to as 'the gap' (between the pixel contact and steering electrode). To find the optimal anode contact geometry, we have divided the anode plane into four quadrants of 4 x 4 pixels, each having a different gap size. The widths of the gaps in the four quadrants are 100 $\mu$m, 150 $\mu$m, 200 $\mu$m and 250 $\mu$m. In all four quadrants, the common grid of steering electrodes is 50 $\mu$m wide. The CdZnTe crystal is indium-bump bonded to a low-noise VLSI circuit for read-out. The cathode on the opposite side is exposed to the source of illumination.

III. PHENOMENOLOGY OF CHARGE-SHARING

We refer the readers to our earlier papers \cite{2} for the analysis of single-pixel events in our detector. We now summarize the observations from our study of charge-sharing events.

A. Our charge-sharing experiment

In our charge-sharing experiment, we placed a collimated source of $^{241}$Am above two adjacent pixels (denoted 1 and 2) in the detector, and measured the pair of pulse heights, $(E_1, E_2)$, induced at the pixels. We set the bias voltage at the cathode to $HV = -250$ V relative to ground at the anode, and the grid of steering electrodes to various values between $V_{\text{steer}} = -16$ V and $-10$ V. The ambient temperature was about 13°C. Both pixel 1 and 2 were in the quadrant with gap size 150 $\mu$m. First, we positioned the collimated source at the centre of pixel 1, measured the pulse height induced, and obtained an energy spectrum, $S_1$, of single-pixel events at pixel 1. Next, we did the same steps at pixel 2, obtaining spectrum $S_2$ of single-pixel events at pixel 2. Then, we placed the collimated source
midway between the centres of the two pixels, and measured pairs of pulse heights, \((E_1, E_2)\), in this configuration, in which most events are charge-sharing. Finally, we drew a scatter plot of \(E_2\) against \(E_1\) for all charge-sharing events in our data. We performed this sequence of steps repeatedly as we vary the potential at the steering electrodes from \(-10\) V to \(-16\) V, in increments of \(-2\) V, producing a series of \(E_2\) against \(E_1\) scatter plots.

The issue of energy calibration requires some special explanation. To calibrate the energy scale of \(E_1\), we took the 59.5-keV spectral line of \(^{241}\)Am as reference, and measured its corresponding pulse height in the single-pixel event spectrum \(S_1\). This gave us a conversion factor between the pulse height and energy, which we applied to obtain the \(E_1\) values, assuming that the signal gain at pixel 1 did not change as we moved the collimated source from the centre to the edge of the pixel. To calibrate the \(E_2\) values, we went through the same procedure using the \(^{241}\)Am line in spectrum \(S_2\).

B. Observations from our experiment

Figure 2 shows a typical plot of the energy-calibrated pulse heights, \(E_2\) against \(E_1\), in charge-sharing events between two pixels, as observed in our detector. The ‘track’ diagonally across the plot represents pairs of pulse heights from the 59.5-keV photons in charge-sharing events. The two square symbols, joined together by a solid line, indicate the reference points at \(E_1, E_2 = 59.5\) keV, as obtained from spectra \(S_1\) and \(S_2\). The triangular symbols, also joined by another solid line, indicate the pulse height positions for single-pixel events measured when the collimated source is in between the pixels. We have identified three main features in these graphs:

1. ‘Parallel shift’ of the ‘track’: For both pixels, the pulse height measured for single-pixel 59.5-keV photons is lower when the collimated source is at the edge of the pixel than when it is at the centre. Thus, there is an apparent shift to lower energies in single-pixel events occurring near the edge of the pixel, compared to those near the centre (this is also the reason for our previously described method of energy calibration when the source is in between the pixels).

2. ‘Curvature’ of the track: In charge-sharing events, if all charges are collected by either of the pixels, then the sum of the pulse heights, \(E_1 + E_2\), should be equal to that in single-pixel events. In other words, the track of data points should coincide with the straight line joining the triangular symbols in Figure 2. This is clearly not the case for our data, as observed in the figure. The curvature of the track implies that more energy is unaccounted for—i.e., more charges are lost—when \(E_1\) and \(E_2\) are comparable than when they are not. Note that this effect pertains only to charge-sharing events, and is distinct from the ‘parallel shift’ we have just discussed, which affects both single-pixel and charge-sharing events.

3. Escape photon ‘kinks’: Rather than appearing as a narrow line, the track appears as a broad distribution of points, extending to two ‘kinks’ at \((E_1, E_2) \approx (25\) keV, 35 keV) and \((35\) keV, 25 keV) on the high energy side. We note that one of these values, 25 keV, is close to the energies of the K-shell electron in cadmium (23.2 and 26.1 keV) and tellurium (27.5 and 31.0 keV), and that the energies in each pair sum to 59.5 keV, the \(^{241}\)Am photon energy. We attribute this phenomenon to the escape of the K-shell photon, produced as the atom de-excites after the initial photoelectric interaction. The mean free path of these K-shell photons ranges from 60 to 135 \(\mu\)m, which is a reasonable fraction of the pixel size of our detector. Thus, it is possible for the K-shell photons to not be deposited in the same pixel, resulting in the observed distribution of points along the track in Figure 2.

It is clear from observations 1 and 2 that in charge-sharing events in our CdZnTe detectors, the induced pulse height do not completely account for the energy of the incident photon. In other words, the problem of charge loss for events near the gaps in the CdZnTe crystal degrades the spectral resolution of our detector. In order to understand this charge-sharing phenomenon, which may shed light on ideas to improve the spectral resolution, we have developed numerical models to study the processes of charge transport within our CdZnTe detector. We now describe the latest version of our model and the results obtained thus far.

IV. OUR NUMERICAL MODEL

In our CdZnTe model, we emphasize on emulating the physical process of charge transport. To simplify the computation in the first stage of our analysis, we assume that the effects of drift and diffusion can be considered separately, and combined at the end. Currently, we concentrate on studying the effects of drift. To do so, we calculate the electric and weighting fields within our CdZnTe detector, by solving the three-dimensional Poisson’s equation numerically on a rectangular grid of Cartesian coordinates. We set the cathode and anode planes parallel to the xy-plane, and represent each
pixel by 40 x 40 grid points. In the perpendicular z-direction, 80 grid points cover the 2 mm depth of the CdZnTe crystal, and an additional 10 cover the 0.8-μm layer of air between the anode plane and the VLSI back plane. To simplify and speed up our calculation, we model our pixels as a 3 x 3 array of 667 μm x 667 μm square pixels, instead of the 8 x 8 rectangular ones of similar dimensions in reality. As for boundary conditions, we assume the steering electrodes surrounding our 3 x 3 array of pixels to extend outward infinitely. The models we use are modified versions of programmes originally used for modelling charge transport in Ge detectors [4, 5]. The algorithm we use to solve Poisson's equation is the Gauss-Seidel method with 'simultaneous over-relaxation,' as described by Press et al [6, § 17.5]. Note that we convert the equations given by Press et al into their equivalents in three dimensions. All derivatives are approximated by first-order finite differences. The boundary condition at the gap is set by the conservation of surface and bulk leakage currents. Having obtained the electric and weighting potentials from Poisson's equation, we calculate their gradient fields by using fourth-order finite differences to approximate the derivatives (third-order at the boundaries between CdZnTe and the metal electrodes, using only potential values on the CdZnTe side). This gives us accurate determination of the weighting field, \( \tilde{W}(\vec{x}) \), as well as the electric fields, \( \vec{E}(\vec{x}) \), for any combination of biases we apply on the cathode and the steering electrodes.

With the fields determined, we find the trajectories of charges (electrons and holes) within our detector. As the starting positions of the trajectories, we pick a set of points that covers the xy-plane at the depth of 256 μm from the cathode plane, the mean free path of 59.5 keV photons in CdZnTe. We then trace the charges in constant spatial steps (as opposed to constant time steps) of length \( |d\vec{x}| = 0.1 \mu m \) in the direction of the electric field lines; we find the field in between grid points by trilinear interpolation. At each step, we compute the contribution of the step to the signal induced at the anodes as \( q_i \tilde{W}(\vec{x}) \cdot d\vec{x} \), where \( q_i \) is the amount of charge as traced at step \( i \). The sum of these contributions along a trajectory thus gives the signal induced at each pixel due to the charge along that trajectory. We also account for the trappings of charges in CdZnTe by modifying \( q_i \) after each step, so that for electrons, \( q_{i+1} = q_i \exp \left( -\frac{|d\vec{x}|}{\lambda_n(\vec{x})} \right) \), where \( \lambda_n(\vec{x}) = v_n(\vec{x})\tau_n \) is the mean free path of electrons in CdZnTe, \( \tau_n \) the mean trapping time, and \( v_n(\vec{x}) \) the drift velocity. We assume that the drift velocity is not saturated, so that \( v_n(\vec{x}) = \mu_n |\vec{E}(\vec{x})| \), where \( \mu_n \) is the electron mobility in CdZnTe. The same formula applies for holes, with the corresponding hole parameters. We have determined from experiments the value of \( \mu \tau \) for our detectors to be \( 1.5 \times 10^{-3} \) cm/V for electrons, and \( 1.0 \times 10^{-5} \) cm/V for holes. In addition, we allow for different values of \( \mu \tau \) at the detector surface, to account for the possibility of increased trapping. By tracing all trajectories from the 256 - μm photon interaction depth to the cathode and anodes, we know the signal induced, \( E_i(\vec{x}) \), at each pixel \( i \), as a function of the starting position, \( \vec{x}_i \), of the drift.

So far in our calculations, we have only considered drift. At this point, we incorporate the effect of diffusion by the following method. For each starting position \( \vec{x}_0 \), we weigh the signal induced, \( E_i(\vec{x}) \), by a two-dimensional Gaussian distribution of starting positions (in the xy-plane) centred at \( \vec{x}_0 \). Then, we sum all the weighted signals to give the pulse height measured at pixel \( i \), due to a photon interaction at \( \vec{x}_0 \) (in practice, we implement this as the convolution of \( E_i(\vec{x}) \) with the Gaussian distribution). The Gaussian distribution represents the charge cloud produced by diffusion; we set its width to be \( \sigma_x = \sigma_y = 26 \mu m \), which we measured from experiment. Finally, we plot pairs of the convolved pulse heights measured at adjacent pixels and due to the same photon interaction against each other; we then compare resulting plot with pulse-height plots obtained experimentally, such as the one shown in Figure 2.

V. RESULTS AND DISCUSSION

For illustrative purpose, we show the result of our electric field calculation (for \( V_{steer} = 10 \) V) in Figure 3. Note that far from the anode plane, the field lines are essentially straight lines. Figure 3 also shows the structure of the electric field near the low-field region adjacent to a steering electrode; from our model, we find the lowest field strength to be 102 V/cm, while the field in the bulk of the detector is on the order of 1 kV/cm.

From our information of the pulse heights at each pixel induced by a given charge trajectory, we are able to classify the pixel plane into regions of photon interaction, producing single-pixel events, or 2-, 3- or 4-pixel coincidence. This allows us to estimate the proportion of each type of event, assuming constant efficiency across the detector, when an uncollimated source illuminates the entire detector. These regions are shown in Figure 4. For \( V_{steer} = 10 \) V, and with a 2σ event threshold, 64% of all events should be single-pixel events, 33% are 2-pixel coincidence, while 3- and 4-pixel coincidences are 1.5% each. This shows that charge-sharing events, which contributes about one-third of all detections, is significant in our detector application. In order to recover useful spectral information from these events, a clear understanding of charge sharing is essential.

Figure 5 shows a major result of our calculation—a plot of the pulse heights at adjacent pixels in charge-sharing events,
scatter plot of the experimental data, we superpose the curve obtained from our numerical model, marked by crosses along its length. Each cross indicates a data point obtained from a given starting position of the drift. Having eight crosses on the curve indicates that both pixels are triggered only when the initial photon interaction occurs within seven grid spacings at the boundary of the pixels, ie, 117 μm, or when ±2.24σ of the charge cloud intersects the pixel boundary. As the calculated curve lies on the higher energy side of the 'track', it is apparent that our model, with no free parameter, predicts lower charge loss than our measurements indicate. To account for this discrepancy, we vary the value of μτ on the surface of the CdZnTe crystal, as mentioned in section IV, and find the value of the ratio \( \frac{\langle \mu \tau \rangle_{\text{surface}}}{\langle \mu \tau \rangle_{\text{bulk}}} \) that makes the model and the data agree. Figure 6 shows the variation in the calculated curve as \( \frac{\langle \mu \tau \rangle_{\text{surface}}}{\langle \mu \tau \rangle_{\text{bulk}}} \) varies between 0 and 1. As Figure 6 indicates, the amount of charge loss is very sensitive to the value of \( \langle \mu \tau \rangle_{\text{surface}} \). This is to be expected, as the weighting field is strongest near the anode plane, so that the induced signal is also the most dependent on the drift of the charges in this region. Unfortunately, there is yet no method to accurately determine this quantity experimentally. Our attempt to measure it indicates that \( \frac{\langle \mu \tau \rangle_{\text{surface}}}{\langle \mu \tau \rangle_{\text{bulk}}} \approx 0.25-25% \). On the other hand, by finding the values of \( \langle \mu \tau \rangle_{\text{surface}} \) that make our modelling results agree with the experimental data, we are able to produce independent estimates of \( \langle \mu \tau \rangle_{\text{surface}} \), which are given in Table 1. We must emphasize that when obtaining these estimates, we fit the calculated curves to the data by eye only. To exemplify this, we show a series of calculated curves that 'fit' the data in Figure 7. A clear problem exists with the values given in Table 1—if the additional charge loss is indeed solely due to reduced μτ on the CdZnTe crystal surface, then \( \langle \mu \tau \rangle_{\text{surface}} \) should be constant, independent of the electric field, and thus the bias applied at the steering electrodes. One possible explanation is that on the crystal surface, the drift velocity saturates, and is no longer proportional to the electric field, violating our assumption. On the other hand, there can also be other yet unaccounted effects that cause additional charge loss. In particular, our simplified treatment of diffusion may not be sufficient to account for its entire effect. We note in particular that as the charges pass through the low-field region below the steering electrode shown in Figure 3, diffusion may cause charge to enter and be trapped there, causing additional charge loss. We have roughly estimated the drift velocity there to be still about ten times greater than the diffusion speed. Yet,
VI. CONCLUSION

In this study, we have demonstrated that our numerical model, which stresses a physical picture of the charge transport processes and an accurate calculation of the drift, can reproduce the general trend of the charge-sharing scenario in our CdZnTe detectors. Our calculation has also yielded estimates of the surface \( \mu \tau \) of our CdZnTe detector, as shown in Table 1. However, more effort is needed in order to account for the exact amount of charge loss measured in our experiments. The next step in our modelling effort is thus to study diffusion in a more detailed analysis, so that an integrated understanding of drift and diffusion in our detectors can be reached.

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VIII. REFERENCES


