Numerical Modelling of Charge-Sharing in CdZnTe Pixel Detectors

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Abstract—In this paper, we describe charge collection in CdZnTe pixel detectors, with emphasis on events split between multiple pixels (charge-sharing events). We describe the design of the CdZnTe pixel sensors, being developed for the balloon-borne High Energy Focusing Telescope (HEFT), and discuss investigations of charge sharing between pixels. We have developed a numerical model which emulates the physical processes of charge transport within the CdZnTe crystal. We discuss this numerical model in detail here. With this model, we are able to reproduce the general features of charge-sharing events. We have found that the amount of charge loss is very sensitive to the surface $\mu r$ (the product of charge mobility and trapping time), and we present estimates of $[\mu r]_{\text{surface}}$ derived 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

O UR group at the California Institute of Technology has been developing CdZnTe pixel detectors for use in astrophysical applications, and specifically, the balloon-borne High Energy Focusing Telescope (HEFT) [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 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 an earlier paper [2] we reported studies of the 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 subsequent effort to study charge-sharing events—events in which photons are absorbed in between pixels, inducing charges on two or more pixels. The phenomenon of charge-sharing has been studied by other groups, for both CdZnTe [3] and silicon detectors [4]. Previous studies of charge-sharing in the HEFT detectors were described in Bolotnikov et al [5]. Here, we 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

The prototype HEFT CdZnTe detector, shown in Fig. 1, contains an array of $8 \times 8$ pixels. The pixel pitch has dimensions $680 \mu m \times 650 \mu m$ (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 Fig. 1. At the centre of each pixel is a rectangular metal contact for the anode, held at ground potential. At the perimeter, the pixel contact is surrounded by a 'steering electrode', held at a negative potential relative to the anode. The steering electrodes of all pixels are connected into a grid, as shown in Fig. 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 investigate the effect of different gap geometries, we have divided the anode plane into four quadrants of $4 \times 4$ 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 at the anodes to a low-noise VLSI circuit for read-out. On the opposite side, the cathode plane is irradiated with X-rays.

![Fig. 1. The anode-plane configuration of the CdZnTe detector.](image-url)

The VLSI chip provides, for each pixel, a complete precision analog signal processing chain, including a charge sensitive preamplifier, shaping amplifier and a peak detect and hold circuit. For a $40 \mu s$ peak time setting and simulated...
detector leakage near 0.1 pA, the measured noise referred to the input is equivalent to approximately a 0.25 keV FWHM energy loss (or about 30 electrons) in the CdZnTe crystal. More details on the circuitry and performance of the chip can be found in Cook et al. [6].

III. PHENOMENOLOGY OF CHARGE-SHARING

We refer the readers to an earlier paper [2] for the analysis of single-pixel events in this CdZnTe pixel detector. We now summarize the observations from studies of charge-sharing events.

A. Experimental setup

To investigate charge-sharing events, we placed a collimated source of $^{241}$Am on the cathode side of the detector, opposite to two adjacent pixels (denoted 1 and 2 in Fig. 1) on the anode side, and measured the pair of pulse heights, $(E_1, E_2)$, generated at the pixels at each event. 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 $V_{steer} = -16$ V and $-10$ V. The ambient temperature was about 13°C. Both pixel 1 and 2 are in the quadrant with gap size 150 μm. First, we positioned the collimated source at the centre of pixel 1, measured the pulse height generated at each event, 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 the charge from most events is shared between pixels. 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, varying 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. We found that in single-pixel events, the 59.5-keV spectral line of $^{241}$Am appeared as a much wider line and at lower channels when the source is collimated between the pixels (i.e., when all $(E_1, E_2)$ are measured) than when it is collimated at the centre of either (when $S_1$ and $S_2$ are measured). Fig. 2 shows the relevant spectra. This observation prompted us to measure from spectrum $S_1$ the conversion factor between pulse height and energy for pixel 1, and apply it to the $E_1$ values. To calibrate the $E_2$ values, we went through the same procedure using the $^{241}$Am line in spectrum $S_2$ as the reference. This change in pulse height is further discussed in Section III-B below.

B. Observations from our experiment

Fig. 3 shows a typical plot of the energy-calibrated pulse heights, $E_2$ against $E_1$, for charge-sharing events. The ‘track’ diagnostically 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 method of energy calibration when the source is in between the pixels, as described at the end of Section III-A above).

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 Fig. 3. 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 $(E_1, E_2) \approx (25 \text{ keV}, 35 \text{ keV})$ and $(35 \text{ keV}, 25 \text{ keV})$ 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 $^{241}\text{Am}$ 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 Fig. 3.

It is clear from observations 1 and 2 that in charge-sharing events, the measured pulse height does not completely account for the energy of the incident photon. In other words, charge loss for events near the gaps in the CdZnTe crystal degrades the detector spectral resolution. While we have plotted only the results for pixels 1 and 2 here, the same results are repeatable at other pairs of pixels in all four quadrants. In order to understand the detailed charge transport for charge-sharing events, which may shed light on ideas to improve the spectral resolution, we have developed a numerical model of the detector. We now describe the latest version of the model and the results obtained thus far.

IV. THE NUMERICAL MODEL

The numerical model emulates the transport of electrons and holes in the detector. To simplify the computation in the first stage of analysis, we assume that the effects of drift and diffusion can be considered separately and combined at the end. We calculate the electric and weighting fields within the 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 8-μm layer of air between the anode plane and the VLSI back plane. For simplicity and speed, we model the pixels as a 3 x 3 array of 667 $\mu$m x 667 $\mu$m 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 the 3 x 3 array of pixels extend to infinity. The models are modified versions of programmes originally used for modelling charge transport in germanium detectors [7], [8]. The algorithm we use to solve Poisson’s equation is the Gauss-Seidel method with “simultaneous over-relaxation”, as described by Press et al. [9, § 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, $\vec{W}(\vec{x})$, as well as the electric fields, $\vec{E}(\vec{x})$, for any combination of biases we apply on the cathode and the steering electrodes.

Besides the fields, the drift of charges in the detector also depends on their mean free paths, $\lambda_{\text{drift}}(\vec{x})$, in CdZnTe. For electrons (n), $\lambda_{\text{drift}}(\vec{x}) = v_n(\vec{x})\tau_n$, where $\tau_n$ is the mean trapping time and $v_n(\vec{x})$ is the local drift velocity. From earlier experiments [10], we have found that the drift velocity is not saturated up to field strengths of at least 3.0 kV/cm, so that $v_n(\vec{x}) = \mu_n|\vec{E}(\vec{x})|$, where $\mu_n$ is the electron mobility in CdZnTe. The same formulate apply for holes (p), with the corresponding hole parameters. We have determined from the same experiments [10] the value of $\mu_p$ for our detectors to be $1.5 \times 10^{-3}$ cm$^2$/V for electrons, and $1.0 \times 10^{-2}$ cm$^2$/V for holes. In this model, we allow for different values of $\mu$ at the detector surface, to account for the possibility of increased trapping. The presence of crystal surface defects that inhibit charge transport is well-known in other semiconductor material such as silicon, so we expect to see similar effects in CdZnTe as well. As one measures the product $\mu\tau$ together experimentally, $(\mu\tau)_{\text{surface}}$ serves as a convenient indicator of the charge transport quality on the crystal surface. In this model, we use $(\mu\tau)_{\text{surface}}$ instead of $(\mu\tau)_{\text{bulk}}$ only on the anode plane; i.e., this surface has no thickness in the z-direction.

With the fields and $\mu\tau$ determined, we next find the charge (electrons and holes) trajectories. We start tracing charges at a depth of 256 $\mu$m (the mean free path of 59.5 keV photons in CdZnTe) from the cathode plane. We cover this xy-plane uniformly with 40 x 40 starting positions for each pixel, displaced from the electric field grid nodes (described earlier in this section) by half the grid spacing in both the x- and y-directions. We then trace the charges in...
constant spatial steps (as opposed to constant time steps) of length $|\Delta x| = 0.1 \mu m$ 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 traced charge to the charge induced at the anodes as $dq_i(x_i) = q_i \hat{W}(x_i) \cdot d\hat{x}_i$, where $q_i$ is the amount of charge traced at step $i$, between $x_i$ and $x_i + d\hat{x}_i$. The sum of these contributions along a trajectory thus gives the charge induced at each pixel due to the charge traced along that trajectory. We also account for charge trapping by modifying $q_i$ after each step, so that for electrons, $q_{i+1} = q_i \exp \left[ -\frac{|d\hat{x}_i|}{\lambda (x_i)} \right]$, where $\lambda_n(x_i) = \nu_n(x_i) \tau_n = \mu_n \tau_n |\hat{E}(x_i)|$, as described in the previous paragraph. If the electric field guides an electron to land on the bare CdZnTe surface on the anode plane, the $\mu r$ value is modified from $\mu r_{\text{bulk}}$ to $\mu r_{\text{surface}}$, and tracing continues along the CdZnTe surface until an anode is reached. By tracing the holes and electrons on all trajectories from the photon interaction depth (at 256 $\mu m$ from the cathode plane) to the cathode and anodes respectively, we know the total charge induced, $Q_j(x_0) = \sum_i dq_j(x_i) = \sum_i q_i \hat{W}(x_i) \cdot d\hat{x}_i$, at each pixel $j$, as a function of the starting position, $x_0$, of the drift (with $q_i = q_{i-1} \exp \left[ -\frac{|d\hat{x}_i|}{\lambda (x_i)} \right]$, as shown above). To convert $Q_j(x_0)$ into energy values $E_j(x_0)$, we pick the trajectory that goes through the centre of the pixel, and let the charge induced due to this trajectory, $Q^*$, correspond to the incident photon energy, namely 59.5 keV. Thus, $E_j(x_0) = (59.5 \text{ keV}) \frac{Q_j(x_0)}{Q^*}$. This conversion method is consistent with the energy calibration in our experiment, as described at the end of Section III-A.

So far we have only considered drift. We incorporate the effect of diffusion by the following method: For each starting position $x_0$, we weigh the pulse height function, $E_j(x)$, by a two-dimensional Gaussian distribution of starting positions (in the xy-plane) centred at $x_0$. Then, we sum all the weighted pulse heights to give the pulse height measured at pixel $j$, due to a photon interaction at $x_0$ (in practice, we implement this as the convolution of $E_j(x)$ with the Gaussian distribution). The Gaussian distribution represents the charge cloud produced by diffusion; we set its width to be $\sigma_x = \sigma_y = 26 \mu m$, an estimate from experiments [10] and from the Einstein relation. Finally, we plot pairs of the convolved pulse heights measured at adjacent pixels due to the same photon interaction against each other. We then compare the resulting plot with pulse-height plots obtained experimentally, such as the one shown in Fig. 3.

V. RESULTS AND DISCUSSION

We show the result of the electric field calculation (for $V_{\text{steer}} = -10 \text{ V}$) in Fig. 4. Note that far from the anode plane the field lines are essentially straight lines. Fig. 4 also shows the structure of the electric field near the low-field region adjacent to a steering electrode. 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 $kV/cm$. Also according to the model, a 10 $V$ difference across the ‘gap’ suffices only

![Cross-section of the CdZnTe detector showing the electric field and potential near the anode plane.](image-url)

Fig. 4. Cross-section of the CdZnTe detector showing the electric field and potential near the anode plane.
measurements indicate. To account for this discrepancy, we vary the value of $\mu r$ on the surface of the CdZnTe crystal, as mentioned in Section IV, and find the value of the ratio $\frac{\langle \mu r \rangle_{\text{surface}}}{\langle \mu r \rangle_{\text{bulk}}}$ that makes the model and the data agree.

Fig. 7 shows the variation in the calculated curve as $\frac{\langle \mu r \rangle_{\text{surface}}}{\langle \mu r \rangle_{\text{bulk}}}$ varies between 0 and 1. As Fig. 7 indicates, the amount of charge loss is very sensitive to the value of $\langle \mu r \rangle_{\text{surface}}$. This is to be expected, as the weighting field is strongest near the anode plane, so that the induced charge is also the most dependent on the drift of the traced charges in this region. Unfortunately, there is yet no method to accurately determine this quantity experimentally. On the other hand, by finding the values of $\langle \mu r \rangle_{\text{surface}}$ that make our modelling results agree with the experimental data, we are able to produce independent estimates of $\langle \mu r \rangle_{\text{surface}}$, given in Table I.

![Fig. 5. Regions corresponding to single-pixel and coincidence events at the corners of four adjacent pixels. The number of pixels triggered is labelled in each region. The rows and columns of crosses indicate the starting positions of charge trajectories; 40 x 40 trajectories cover this (667 μm)² plane. Also shown in shade are the positions of gaps between the anodes and the steering electrode grid.](image)

![Fig. 6. Comparison of charge loss scenarios as predicted by our model and as observed in experiment. The model assumes $\langle \mu r \rangle_{\text{surface}} = \langle \mu r \rangle_{\text{bulk}}$. The experimental data are the same as the ones shown in Fig. 3; the line marked with crosses along its length is the modelling result.](image)

![Fig. 7. Variation in the extent of charge loss computed with $\frac{\langle \mu r \rangle_{\text{surface}}}{\langle \mu r \rangle_{\text{bulk}}}$ varied between 0 and 1. Curves shown are for $\frac{\langle \mu r \rangle_{\text{surface}}}{\langle \mu r \rangle_{\text{bulk}}}$ = 0, 0.05, 0.10, 0.16, 0.40 and 1.0.](image)

**TABLE I**

<table>
<thead>
<tr>
<th>$V_{steer}$</th>
<th>$\frac{\langle \mu r \rangle_{\text{surface}}}{\langle \mu r \rangle_{\text{bulk}}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>-10 V</td>
<td>9-10%</td>
</tr>
<tr>
<td>-12 V</td>
<td>14-17%</td>
</tr>
<tr>
<td>-14 V</td>
<td>17-30%</td>
</tr>
</tbody>
</table>

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 Fig. 8.

A clear problem exists with the values given in Table I—if the additional charge loss is indeed solely due to reduced $\mu r$ on the CdZnTe crystal surface, then $\langle \mu r \rangle_{\text{surface}}$ should be constant, independent of the electric field, and thus the bias applied at the steering electrodes. We believe this problem can be caused by some charge loss mechanism yet unaccounted by this model. The $\langle \mu r \rangle_{\text{surface}}$ estimates here may well be ‘effective values’ only, shielding other charge loss effects. Potential causes include the possibility that on the crystal surface, the drift velocity saturates, and is no longer proportional to the very strong electric field at the gap (contrary to our assumptions). On the other hand, the trapping time may also depend on the field in some unknown manner. While we may be able to dismiss the problem by introducing various surface defects in the model, we are reluctant to incorporate any feature that is not undis-
putably observable in experiments. However, we do think that 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 Fig. 4, 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, more detailed study of the effects of diffusion will be needed, and this will be the next step in extending our numerical model.

VI. CONCLUSION

In this study, we have demonstrated that a simplified numerical model of the charge transport processes can reproduce the general trend of the charge-sharing in CdZnTe pixel detectors. Our calculation has also yielded estimates of the surface $\mu r$ of our CdZnTe detector, as shown in Table I. However, more effort is needed in order to account for the exact amount of charge loss observed experimentally. The next step in our modelling effort will be to study diffusion in a more detailed way, so that we can reach a complete understanding of drift and diffusion in CdZnTe pixel sensors.

VII. ACKNOWLEDGMENT

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REFERENCES


