Charge Transport Optimisation in CZT Ring-Drift Detectors

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Abstract. Ring-Drift design has been applied to large ($7.5\text{mm} \times 7.5\text{mm} \times 2.3\text{mm}$) Cadmium Zinc Telluride (CZT) devices. This low-noise, single-carrier-sensing configuration is the gold standard for spectroscopic silicon X-ray detectors. By combining the advantages of Ring-Drift with the high quantum efficiency and room-temperature operating capabilities of CZT, a simple and compact device for high-resolution spectroscopy of X-rays in the range 50-500keV can be created. Quality of CZT crystals has improved greatly in recent years and electron-only sensing overcomes the problem of inherently poor hole transport in II-VI semiconductors.

The spatial response of our 3-ring CZT device was studied by microbeam scanning while the voltages applied to all electrodes were systematically varied. Maximum active radius extended to 2.3mm, beyond the second ring. Resolution was limited by electronic noise. Our results show that the lateral field and its ratio to the bulk field exert a crucial influence on active area, peak position and sensitivity. CZT and the device geometry were modelled in 3D with Sentaurus TCAD. Line scans were simulated and trends in performance with bias conditions matched experimental data, validating the model. We aimed to optimise the resolution, sensitivity and active radius of the device. Fields and charge drift were visualised and the active volume was mapped in 3D to improve understanding of the factors governing performance including number of rings, their widths, positions and bias.

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Figure 1. Prototype detector electronic layout with 0.5mm ring and gap widths

1. Introduction

Cadmium zinc telluride (CZT) is increasingly used for room temperature spectroscopy of 50-500keV X-rays in many fields including medical and industrial imaging, the nuclear industry and astrophysics [1]. CZT is desirable as a replacement for cryogenically-cooled HgGe because its wide band gap (1.6eV) permits room temperature operation. Poor charge transport limits the performance of CZT crystals: in particular, hole mobility is an order of magnitude lower than electron mobility. Trapping of holes leads to incomplete charge collection and low-energy ‘tailing’ at peaks [2]. ‘Drift’ geometry is among the most effective for single-carrier (electron) sensing [3,4]. Drift design has two defining properties: the bulk is fully depleted and electrons are steered towards the anode by a lateral drift field via suitably biased electrodes [5]. ‘Linear’ drift designs have a strip anode and parallel strip steering electrodes; ‘Ring-Drift’ devices commonly have a central anode with concentric rings of steering electrodes covering one face and a solid cathode covering the other [6]. Silicon ring-drift detectors have lower noise than any other configuration for a given active volume owing to the minimal anode area [7]. They are the standard for XRF mapping, scanning electron microscopes, particle physics and many other X-ray applications [8–11].

The potential advantages of Ring-drift design in CdTe-based semiconductors have begun to excite interest. It is desirable to replicate the excellent spectroscopic performance of silicon devices in a material with higher quantum efficiency for hard X- and gamma rays. Crystals grown by the Travelling Heater Method (THM) have recently become available and show evidence of superior spectroscopic qualities compared with previous material [12–14].

The first CZT linear drift detector (1998) proved an effective single-carrier sensor [15]. The design was developed further for high-energy astrophysics [16,17]. The first approach to CZT ring-drift had only a point anode and guard ring on the anode face extending to the 3mm^3 wafer edge, with no intermediate rings. Cathode and guard ring voltages were equal (-500V relative to the anode). Resolution equalled or improved upon that of all other CZT devices at the time [18,19].

Multiple-ring configuration did not appear until 2007 [20,21]. This 1.1mm-diameter device displayed complex variations in sensitivity with interaction position, applied bias and photon energy.

Our group has previously studied a CdTe 3-ring device 1mm thick and 7.5mm in diameter [22] with radioisotope sources (59.5keV - 662keV) and microbeam scanning. Active radius and sensitivity increased with lateral field but leakage noise limited performance. In this work we present a microbeam study of a 2.3mm-thick CZT device of the same ring geometry (figure 1). The higher resistivity of CZT permits greater field strengths without loss of resolution, resulting in greater active area as well as improved efficiency [23].

We have modelled the electronic properties of CZT device in 3D and simulated experimental linescans to validate the model. Synopsys Technology CAD (TCAD) is a powerful tool with extensive visualisation capabilities that has already proven invaluable for semiconductor detector development [24]. We have varied ring number, width, position and bias conditions in the search for optimum energy registration, active area and sensitivity. Fields and charge trajectories for many interaction positions have been studied to inform the optimisation process and aim to identify which physical processes limit predicted performance.

2. Synchrotron Microbeam Linescans of Prototype

The electrode layout in figure 1 was sputtered on a THM-grown CZT wafer $10\text{mm} \times 11\text{mm} \times 2.3\text{mm}$. The ring face was bump-bonded to custom-shaped gold-plated contacts on a ceramic tile using conductive adhesive by the STFC Rutherford Appleton Laboratory (RAL). The planar gold cathode was wire-bonded at the corner of the wafer. A four-channel power supply (ORTEC 710) biased the rings and cathode independently at up to -1000V such that the bulk and lateral (‘drift’) fields could be varied. The guard ring floated to an unknown potential and the anode was grounded through an Amptek CoolFET A250 charge sensitive preamplifier. An ORTEC 570 shaping amplifier, ORTEC 480 pulse generator and Canberra 9635 Analogue-to-Digital Converter (ADC) and Canberra

Figure 2. (a) Anode spectra of 3-ring prototype CZT drift detector undergoing radial linescan. (Ring 1, Ring 2, Ring 3) Cathode = (-500,-600,-700)-700V. (b) Plot of peak centroid energies as a function of radial position of incident microbeam. Spectra recorded at $10\mu\text{m}$ intervals.

Multi-Channel analyser (MCA) were used.

The cathode face of the detector was irradiated with a $20\mu\text{m} \times 20\mu\text{m}$ microfocus synchrotron beam at the Diamond Light Source [25]. The X-ray energy was controlled by a Si(1 1 1) double crystal monochromator, with a fundamental energy of 25keV and a beam of 2×10^5 photons s^{-1} . Aluminium absorbers 12.5mm thick reduced the beam to 400 photons s^{-1} at 25keV and 50 photons s^{-1} at the 3rd harmonic energy, 75keV. Spot size was controlled by tungsten slits. The detector box was mounted vertically on a computer-controlled X-Y stage. Linescans were made with 0.1mm steps and 30s acquisition times along one radius. Lateral and bulk fields were systematically varied and the bias scheme

producing the greatest active area was identified. With this scheme, the linescan was repeated with a $10\mu\text{m} \times 10\mu\text{m}$ spot size in $10\mu\text{m}$ steps.

3. Linescan results

Figure 2(a) shows a typical anode spectrum (*black*). Our prototype box and electronic system were not optimised for noise performance and this proved the limiting factor in resolution. High noise occurs below 15keV. FWHM was used as a measure of resolution. The primary beam ($\approx 25\text{keV}$) and the 3rd harmonic energy produced peaks with FWHM of $(5.8 \pm 0.1)\text{keV}$ and $(6.3 \pm 0.1)\text{keV}$ respectively. Measurement of the noise in the readout chain indicate that the FWHM resulting from the detector alone is 2.9keV and 3.8keV respectively [23].

The peak at $\approx 75\text{keV}$ is symmetrical in shape and does not display the ‘hole tailing’ features associated with planar CZT detectors at this energy [2]. The peak at 50keV represents pulse pileup; the 2nd harmonic is forbidden. With low bulk and lateral potential ($< 300\text{V}$), only beam positions over the anode produced spectra of the quality shown in figure 2(a) (*black*). Beyond the anode edge, peaks shifted to lower energies and collapsed. Increasing the lateral field as a fraction of bulk field increased active area and sensitivity. Scaling up both fields caused further improvement, whereas raising the bulk field alone did not. A maximum sensitive radius of 2.3mm was achieved with bias

(Ring 1, Ring 2, Ring 3) Cathode = (-500,-600,-700)-700V (figure 2(b)). The spectrum quality is constant up to 2.3mm radius. Figure 2(a) illustrates the energy spectrum at 2.40mm radius (*grey*) which shows a small shift in peak energies. There are no identifiable peaks beyond 2.50mm, indicating the edge of the detector’s active area. The $\approx 200\mu\text{m}$ radial distance over which counts are registered at incorrect energy is a very small fraction of the total active area. The anode leakage under this bias scheme was $< 10\text{nA}$. Raising the bias to (-600,-700,-800)-800V increased leakage noise but did not increase the active area. Alruhaili *et al.* [23] provide a detailed analysis of all microbeam results.

4. Modelling CZT Material

Detector-grade CZT varies in composition, growth method and in the trap characteristics observed in experiment [26–28]. The mechanisms underlying its electronic properties are not well-understood. It was necessary to create a simple material model with the properties relevant to drift detector performance. A TCAD model of CZT was created by adding traps to a default CdTe model and raising the bandgap

to 1.60eV. Simulations were conducted to identify a trapping scheme that produced realistic resistivity and charge transport, as reported in CZT bulk material [12–14].

4.1. Modelling realistic resistivity

All detector-grade CZT displays high resistivity ρ ($\geq 10^{10}\Omega\cdot\text{cm}$). There must exist a stable compensation mechanism that is effective across all variations in composition.

Previous authors [29,30] have simulated a set of 3 acceptor energies and one or two deep donors, based on experimental data and the supposed physical origins of traps [28,31]. The mechanism by which a deep donor compensates for acceptors involves Fermi level ‘pinning’ [26]. If donor energy E_D is close to the intrinsic Fermi level, large changes in the number of ionised donors correspond to very little shift in the Fermi energy. Altering the concentrations of acceptors, hence the number of free holes to be absorbed by the donor, does not change the Fermi level, provided the reservoir of donors is sufficiently large. The presence of a near-mid-gap level with high concentration explains the high ρ of CZT over many variations in composition.

The current work uses acceptor energies, cross-sections and relative concentrations obtained [14] from a sample of undoped THM-grown CZT (table 1, [30]). I-V simulations were carried out to identify the donor energy and relative concentration N_{Rel} that would result in the most realistic resistivity.

Resistivity exceeds $10^{10}\Omega\cdot\text{cm}$ over the greatest N_{Rel} range for $E_D \approx 0.83\text{V}$. This energy and its N_{Rel} at maximum ρ were chosen for the model. The value of maximum ρ was the same for all donor energies: $1.28 \times 10^{11}\Omega\cdot\text{cm}$.

Resistivity depends only on *relative* concentrations; charge transport properties are determined by *absolute* concentrations. The next task was to identify the set of absolute concentrations that would produce realistic charge transport.

4.2. Modelling realistic charge transport

The significant properties are the mobility-lifetime products of electrons $(\mu\tau)_e$ and holes $(\mu\tau)_h$. These were evaluated by simulating alpha-irradiation of the cathode and anode respectively. $\mu\tau$ was obtained by measuring charge collection efficiency as a function of electric field strength and fitting the Hecht equation to the curve [32]. Field strength was varied from $2.5 \times 10^4\text{V}\cdot\text{m}^{-1}$ to $4 \times 10^5\text{V}\cdot\text{m}^{-1}$.

The cathode of a $2\text{mm} \times 2\text{mm} \times 2\text{mm}$ planar model was ramped from 0V to its operating voltage (50V - 800V) and transient simulation commenced. Current signals were recorded at every timestep. TCAD

Figure 3. (a) Anode current signals following simulated ‘alpha-irradiation of the cathode’ (charge deposition at $10\mu\text{m}$ depth) in a $2\text{mm} \times 2\text{mm} \times 2\text{mm}$ planar CZT detector with 500V bias. Electron and hole mobility-lifetime products $\mu\tau$ were obtained by fitting the Hecht equation to plots of charge collection efficiency against electric field strength. (b) Results: $\mu\tau_e$ and $\mu\tau_h$ as a function of donor concentration N_0 . This plot provided a suitable value of N_0 to complete the CZT material model.

provides a ‘heavy ion model’ for the deposition profiles of common ion species. Any interaction site and time point can be chosen. Time was allowed for the potential field to stabilise and one Am-241 alpha particle was deposited at $10\mu\text{m}$ depth. Simulation continued until all charge motion ceased.

Absolute concentrations of all traps were varied; their relative concentrations were maintained for high resistivity. Donor absolute concentration N_0 is quoted hereafter as shorthand for the set of corresponding acceptor concentrations.

Figure 3(a) shows anode signals following simu-

lated ‘cathode irradiation’, representing electron drift. At $N_0 = 2.5 \times 10^{13} \text{cm}^{-3}$, all charge is trapped at its deposition site within the first few nanoseconds. At $N_0 \geq 2.5 \times 10^{11} \text{cm}^{-3}$ a falling exponential pulse shows that carrier lifetime is shorter than the time required to cross the device. At $N_0 = 2.5 \times 10^{10} \text{cm}^{-3}$, the current declines after its initial peak as some charge becomes trapped. A change in gradient occurs when the remaining cloud is collected. At the two lowest N_0 values, trapping has little effect upon charge transport. A plateau followed by steep decline in current indicates drift and collection of the whole charge cloud. The FWHM of the pulse represents mean drift time across the full width of the device.

$(\mu\tau)_e$ and $(\mu\tau)_h$ were plotted as a function of trap concentration (figure 3(b)). Within error, $(\mu\tau)_e \propto N_0^{-1}$. This results from the trapping model applied by TCAD.

N_D^+/N_D^0 and N_A^-/N_A^0 are the concentrations of ionised/non-ionised donors and acceptors. Capture cross-sections $\sigma_{e,h}$, thermal velocities $v_{th}^{e,h}$ and mobilities are set as constants. The trapping times for a donor level are given by:

$$\tau_{hD} = \frac{1}{\sigma_h N_D^0 v_{th}^h} \quad \tau_{eD} = \frac{1}{\sigma_e N_D^+ v_{th}^e}$$

The trapping times for each acceptor level:

$$\tau_{hA} = \frac{1}{\sigma_h N_A^- v_{th}^h} \quad \tau_{eA} = \frac{1}{\sigma_e N_A^0 v_{th}^e}$$

The cross-sections σ of the donor and the $E_v + 0.48 \text{eV}$ acceptor are some orders of magnitude larger than those of the other acceptors whereas the concentrations N of all four levels differ by a multiple of 25 or less (table 1). The σN product in the denominator of each trapping time equation therefore signifies that the donor and the $E_v + 0.48 \text{eV}$ acceptor level cause the most rapid trapping.

In a deep level ($E_{\text{Trap}} \gg kT$) the residence time is so large that very little de-trapping occurs. Hence the observed relationship $(\mu\tau)_e \propto N_0^{-1}$.

$(\mu\tau)_h \propto N_0^{-1}$ only in the range $N_0 > 2.5 \times 10^9 \text{cm}^{-3}$. Below this concentration, $(\mu\tau)_h$ rises more gradually with falling N_0 . The change in gradient corresponds to the transition from a falling exponential current pulse to a square-topped signal.

The range of experimental values of THM CZT [12–14] $(\mu\tau)_e$ is indicated; $(\mu\tau)_h$ of the same crystals was not reported. A mid-range value of $\mu\tau_e = 3.5 \times 10^{-4} \text{cm}^2/\text{V}$ was selected for the model. The best fit line shows that this requires a donor concentration of $1 \times 10^9 \text{cm}^{-3}$. The corresponding $\mu\tau_h \approx 5 \times 10^{-4} \text{cm}^2/\text{V}$ is somewhat high in comparison with values reported for CZT from other sources ($3 \times 10^{-6} \text{cm}^2/\text{V}$ to

Table 1. Properties of the final model of CZT. Trap concentrations obtained by simulation; energies and cross-sections from a sample of undoped THM-grown CZT [30], [14].

Parameter	Symbol	Value	Units
Bandgap	E_{g0}	1.60	eV
Pair creation energy	W	4.3	eV/ehp
Resistivity	ρ	1.28×10^{11}	$\Omega \cdot \text{cm}$
Electron mobility	μ_e	1.050×10^3	$\text{cm}^2/(\text{Vs})$
Hole mobility	μ_h	8.0×10^1	$\text{cm}^2/(\text{Vs})$
Mobility-lifetime product (electrons)	$(\mu\tau)_e$	3.5×10^{-4}	cm^2/V
Mobility-lifetime product (holes)	$(\mu\tau)_h$	5×10^{-4}	cm^2/V
	Trap energy (eV)	Cross-section (cm^{-2})	Concentration (cm^{-3})
Acceptors	$E_V + 0.08$	1×10^{-17}	4.0×10^7
	$E_V + 0.29$	3×10^{-17}	1.2×10^8
	$E_V + 0.48$	2×10^{-14}	1.0×10^8
Donor	$E_C - 0.83$	1×10^{-10}	1.0×10^9

$1.5 \times 10^{-4} \text{cm}^2/\text{V}$ [14, 26, 33]). However, reported values cover a wide range and it is reasonable to expect a high $(\mu\tau)_h$ for this THM material corresponding to its high $(\mu\tau)_e$. In any case, $(\mu\tau)_h$ is of little significance for testing a single-carrier sensor.

Table 1 summarises the properties of the final model of CZT used in section 5 for device modelling. Values of trap energies and cross-sections, electron and hole mobilities and the bandgap were based on undoped THM-grown CZT [14, 30]. These values were written into the parameter file of default CdTe. Resistivity and $(\mu\tau)_{e,h}$ values emerge during simulation from the specified mobility values, traps and the physical models applied.

5. Modelling Ring-Drift Devices and Simulating Linescans

5.1. Methods

The prototype device (figure 1) was modelled in 3D with perfectly Ohmic gold contacts (figure 4(a)). The ‘heavy-ion model’ was used to simulate X-ray interaction, with the spatial and temporal deposition profile of a 25keV photon undergoing photoelectric absorption in CZT. The 1/e attenuation depth of a 25keV photon in CZT is $70 \mu\text{m}$. This was taken to be a representative depth for replicating a linescan by a series of single-photon simulations at $100 \mu\text{m}$ radial intervals.

3D datasets were recorded at multiple times for visualisation of fields, charge drift and diffusion in any plane (figure 4(b)-(g)). Current signals were integrated to obtain charge collection on each electrode as a function of radius (a ‘Qrad profile’) (figure 5(c)). Active area corresponds to the extent of anode charge

Figure 5. (a) Current signals and (b) Charge signals from the simulation in figure 4 at $r = 2200\mu\text{m}$ (c) Performance is characterised by the anode charge collection as a function of interaction radius. The shape of this radial profile determines the active area and resolution.

collection. A flat response indicates correct energy registration; the region of declining anode charge represents counts registered at too low an energy. The Qrad profile is characteristic of the geometry, bias and interaction depth. To compare the overall performance of devices under uniform illumination, the extent of the flat response must be considered in combination with the loss of resolution caused by partial charge collection. A factor G was devised to quantify spectroscopic quality (Appendix A). The quality factor informed optimisation of the device and its operating conditions.

A variety of field conditions and ring geometries were simulated and interaction depth was varied to represent higher photon energies.

5.2. Comparison of Experimental and Simulation Results

25keV linescans in the prototype device were simulated under the bias conditions used in experiment. Trends in performance were qualitatively reproduced: increasing the lateral field increased active area. Raising ring and cathode voltages with a fixed ratio increased both active area and the maximum value of anode charge collected.

Figure 6 compares linescan data with the simulated Qrad profiles of the anode and Ring 1 under the experimentally optimised scheme of (-500,-600,-700)-700V. The ‘floating’ nature of the guard ring could not be simulated; an applied guard bias of -1000V resulted in spatial performance that most closely matched experimental data. The influence of the guard ring is discussed further in section 5.3.2.

The real device maintains a flat response until beyond Ring 2, indicating that all the charge from each interaction reaches the anode and thus all counts

are registered at the correct energy. The steep decline in peak energy beyond Ring 2 shows that almost no charge from this region reaches the anode.

Modelled anode charge collection declines gradually as some charge is collected by Ring 1. A steep decline occurs beyond Ring 2. The radial range of partial charge collection was large ($> 1000\mu\text{m}$) whereas in experiment the fall from full collection to zero took place over $< 300\mu\text{m}$. In simulation, charge sharing with Ring 1 occurred at all interaction radii beyond its outer edge.

Anode leakage exceeded experimental values by a factor of between 1 and 2 under all bias conditions. Values of leakage in simulation are not reliable because the effects of wafer surface treatments, surface conductivity and bonding to the electrodes are unknown and were not modelled. Unrealistic field conditions close to the surface may also be responsible for the collection of charge on the rings.

5.3. Varying bias conditions, ring geometry and interaction depth: results and discussion

Linescans were simulated under bias conditions outside the experimental range. The aim was to optimise the performance of the model. Qrad profiles were compared with that of the experimentally optimised scheme of (-500,-600,-700)-700V. The models discussed in this section are listed in Table 2 with their quality factor G values.

5.3.1. Effects of varying lateral and bulk bias increments

The relative voltages of the electrodes were systematically altered and trends in Qrad observed.

Firstly, cathode bias was increased while maintaining all ring voltages (figure 7(a) *pink, grey series*)

Figure 4. (a) model of the prototype (figure 1) without a guard ring. (b)-(g) Electron charge cloud after simulated photon interaction at $70\mu\text{m}$ depth, $2200\mu\text{m}$ radius. In this case, charge is shared between the Anode and Ring 1 and a small amount drifts to Ring 2. The resulting electrode signals are shown in figure 5. Bias $(-500, -600, -700) - 700\text{V}$: electrostatic potential is illustrated in figure 8(a).

Figure 6. Comparison of simulated and experimental spatial performance under the optimised experimental bias conditions.

Figure 7. Anode charge collection as a function of radius ('Qrad profiles') of the prototype 3-ring device at $70\mu\text{m}$ interaction depth under various bias conditions (Ring 1, Ring 2, Ring 3) Cathode. (a) The effect of raising bulk voltage alone (solid lines) and of raising inter-ring and bulk voltages (dashed). (b) The effect of raising Ring 1 bias while maintaining inter-ring voltages and Cathode=Ring 3.

This caused a higher uniform response over a smaller area and steeper decline in Qrad. This was as predicted: the larger bulk/lateral field ratio allowed less distance of lateral drift before all the charge reached the anode face. G increased, indicating improved energy resolution. However, the device was scarcely operating in 'drift' mode; charge deposited beyond Gap 1 was almost entirely collected by the rings.

Secondly, inter-ring voltages were increased to 250V, then to 400V. Ring 1 voltage and Cathode=Ring 3 were maintained (figure 7(a), dashed series) produced a similar result. The lateral field close to the cathode remains weak even when there is a large voltage drop across the rings. Charge close to the cathode experienced the high bulk field. Visualisation of the electron cloud showed that its initial trajectory had no lateral component. When it reached a region of high lateral field, it was already too close to the anode face to drift to the anode without being captured by Ring 1.

Thirdly, Ring 1 bias was increased to -800V, then to -1000V. Inter-ring voltages and Cathode=Ring 3 were maintained (figure 7(b)). This resulted in a larger flat-response area but also extended the region of partial charge collection, degrading the overall quality G .

5.3.2. Effects of biasing the Guard ring and scaling all voltages The true voltage of the 'floating' guard used in experiment is unknown. A model with no metallised

Figure 8. Effect of applying a guard ring to the model and varying its bias. (a) Cross-section through model with no guard illustrating electrostatic potential. Equipotentials at 25V intervals.(b) Ditto with a guard biased at -1000V. (c) Qrad profiles at 70μm interaction depth. Biasing the guard causes a steep decline to zero, corresponding to the radius at which the bulk component of the electric field changes direction. Doubling all voltages increases charge collected without altering this radius (*dashed lines*).

guard (figure 8(a)) produced a gradual decline in the anode Qrad profile (figure 7). It was necessary to add a metal guard and impose a voltage to produce a closer match to experimental data (section 5.2). Guard voltages up to -1200V were simulated with the experimentally optimised scheme of (-500,-600,-700)-700V.

A guard more negative than -700V caused the sloping Qrad profile to be ‘cut off’: decline very steeply to zero at a certain radius. This cut-off corresponds to the radius at which the depth component of the electric field falls to zero and changes direction (figure 8(b)

where an equipotential intercepts the cathode). The steep decline in experimental peak energy cannot be ascribed to this field condition because the true floating guard voltage must be smaller than -700V.

A more negative guard decreases this cut-off radius, reducing the active area; a less negative guard increases it, allowing a greater area of partial charge collection. The maximum G (0.59), representing the best compromise between these two effects, was attained with the guard biased at -1000V (figure 8(b), (c) *dashed* ▲).

This bias combination produced the best performance of many simulated schemes with ring, guard and cathode voltages in the range 0 to -1000V. Though some attained higher G with an active radius extending only to Ring 1 (figure 7(a) *solid lines*), this model produced high G while operating as a true ‘drift’ device, collecting the majority of charge deposited within the outer radius of Ring 2.

The next step in optimisation was to scale up all voltages while maintaining the ratio (-500,-600,-700, [-1000])-700V. In experiment, raising ring and cathode voltages with a fixed ratio increased the maximum value of anode charge collected (section 5.2). This trend was reproduced in simulation when voltages were doubled.

In the absence of a guard, the Qrad profile shifted up the charge (Q) axis without significantly altering its shape. The flat-response radius increased very slightly but the range of partial charge collection expanded greatly as charge collection declined gradually to zero from a higher initial plateau. The total effect was to decrease G .

When the guard was biased to cut off the region of partial charge collection at a fixed radius, doubling all voltages improved G as a result of the marginal increase in flat-response radius.

Figure 8(c) (*dashed lines*) illustrates the change in Qrad when doubling (-500,-600,-700, [-1000])-700V: G rose from 0.59 to 0.69. However, anode leakage also doubled from 0.5nA to 1nA. The increase in maximum Q with electric field strength results from the material model (section 4.2): absolute collected charge is limited by carrier lifetime. Faster drift allows a greater proportion of deposited charge to be collected rather than succumbing to traps.

The optimum scale factor depends on the trade-off between improved charge collection and increasing leakage noise. Leakage of 1nA is acceptable in experiment, given the large noise contribution of the readout chain. Simulated leakage current values are not reliable because contact and surface conditions are not modelled (section 5.2). Simulated anode leakage was 1 to 2 times the experimental value under all bias conditions. It was thought reasonable

to seek the optimum bias scheme using the highest voltages possible while maintaining simulated leakage at or below 1nA, on the assumption that even lower leakage current would be observed in experiment. This principle was applied to subsequent studies (sections 5.3.3 and 5.3.4).

5.3.3. Effects of varying ring geometry The 3 rings were narrowed in an attempt to reduce their share of charge collection. The anode and guard radii were kept constant and three 250 μ m rings were placed at the outer edges of the original (500 μ m-wide) ring positions (figure 11(a)). This geometry gave a slightly larger flat-response radius and a shorter range of partial charge collection than the prototype. The value of G rose from 0.69 to 0.78. 250 μ m rings were adopted for all subsequent models.

An uneven electric field slows drift to the anode and increases the probability of trapping and charge collection by the rings [34]. Theory shows that the ratio of drift-strip pitch to wafer thickness should be less than $\frac{1}{2}$ to obtain a sufficiently uniform drift field in the centre of a linear detector. For deep interactions (close to the anode face) even smaller spacing is required. The possible effects of a finer ring structure were investigated by replacing 3 250 μ m rings (750 μ m gaps) with 6 250 μ m rings (Gap 1 750 μ m, other gaps 250 μ m) with the same voltage/distance gradient. Spatial fluctuations in electric field greatly reduced in magnitude. Linescans were simulated at depths from 70 μ m to 1800 μ m. The Qrad profiles of the 3-ring and 6-ring devices showed no significant difference. At $\geq 1800\mu$ m depth, anode charge collection ceased at the inner edge of Ring 1 for both devices. Smoothing the electric field brought no performance benefit.

The drift field was extended over a larger radius, by adding fourth and fifth rings, with the aim of increasing active area. Figure 9 shows one 4-ring geometry under three bias schemes (electrostatic potential plots (a)-(c)) and their Qrad profiles for interactions at 70 μ m depth (d). This 4-ring geometry with bias scheme (a) was created to replicate the best-performing field in a 3-narrow-ring device (figure 11(a)) but extend the active area to a cut-off radius of 3400 μ m. Ring 1 in this geometry has been narrowed to 150 μ m (the very minimum that could be bonded in a real device) and re-positioned repeatedly to minimise its charge collection. However, Qrad profiles show that partial charge collection by Ring 1 affects (a) from $r \approx 1100\mu$ m. $G=0.42$.

Biases were varied to increase the flat-response radius and reduce the range of partial charge collection. A flat response with steep decline was achieved only by moving the cut-off radius so far inwards that the Qrad profile and the electrostatic potential field resembled

Figure 9. (a)-(c) Cross-sections through a 4-ring model showing electrostatic potential under three bias schemes. Equipotentials at 25V intervals. (d) Qrad profiles of models (a)-(c) at 70 μ m interaction depth compared with the best 3-ring model ($G=0.78$). A steep decline to zero in the 4-ring device is only achieved by moving the cut-off radius inside its 3rd ring (c).

that of a 3-ring device: Ring 4 and even Ring 3 became an extension of the guard (figure 9(c),(d), *purple series*. $G=0.60$). None of the large-area 4-ring or 5-ring geometries improved upon the active area or quality achieved with 3 narrow rings and a guard. The aspect ratio of the wafer may be the limiting factor in

maximising active area.

5.3.4. Effects of varying interaction depth The best-performing model tested thus far had 3 $250\mu\text{m}$ rings with $750\mu\text{m}$ gaps and a guard and was biased with the ratio (5,6,7,10)/7 (figure 11(a)). The bias values that would give the best performance in experiment depend upon the trade-off between sensitivity and leakage noise. A reasonable bias scheme of (-1000,-1200,-1400,-2000)-1400V (simulated leakage 1.0nA) was chosen to create a high-resolution 3D map of charge collection (figure 11). The aim was to understand the relationship between potential shape and active volume, enabling more accurate prediction of performance from potential fields and thus quicker optimisation.

Figure 10 illustrates the Qrad at three depths. The steep cut-off observed at $70\mu\text{m}$ (a) is replaced at $1300\mu\text{m}$ depth (b) by a wide radial range of charge sharing. A large negative bias on the guard ring produces a sharp cut-off only for very shallow interactions. At $1800\mu\text{m}$ depth (c) the range of partial charge collection shrinks again as Ring 1 collection dominates. The inner edge of Ring 1 is the limiting active radius. No gaps $> 900\mu\text{m}$ had been used hitherto for reasons described earlier; this data stimulated a study of increasing gap 1 width up to 1750mm by condensing the other gaps or removing one ring.

Figure 11 was constructed by interpolation between ‘linescan’ datasets at 12 depths including those shown in figure 10. The relationship between the potential shape (figure 11 (a)) and partition of charge between electrodes (b)-(e) is evident. At $< 300\mu\text{m}$ depth, anode charge collection extends to the ‘cut off’

Table 2. Quality factor G (Appendix A) of various models undergoing simulated 25keV linescans ($70\mu\text{m}$ interaction depth).

Figure	Bias (V)(R1, R2, R3, (R4), [Guard])Cathode	G
3-ring prototype, no guard		
7(a,b)	(-500,-600,-700)-700	0.43
7(a)	(-500,-600,-700)-1200	0.77
7(a)	(-500,-750,-1000)-1000	0.49
7(b)	(-800,-900,-1000)-1000	0.38
3-ring prototype + guard		
8(b,c)	(-500,-600,-700,[-1000])-700	0.59
8(c)	(-1000,-1200,-1400, [-2000])-1400	0.69
3 narrow rings + guard		
10,11	(-1000,-1200,-1400, [-2000])-1400	0.78
4 narrow rings + guard		
9	(-1000,-1200,-1600,(-2000),[-2200])-1800V	0.42
9	(-1000,-1200,-1400,(-2000),[-2400])-1600V	0.47
9	(-1000,-1400,-1800,(-2200),[-2400])-1600V	0.60

Figure 10. Effect of varying interaction depth. Partition of charge collection between electrodes as a function of interaction radius for the 3-narrow-ring model shown in figure 11(a). Bias (-1000,-1200,-1400, [-2000])-1400V. (a) ‘Linescan’ at $70\mu\text{m}$ depth. $G=0.78$ (b) $1300\mu\text{m}$ depth (c) $1800\mu\text{m}$ depth

radius at which the bulk field (the depth co-ordinate component of the electric field) switches polarity ($\approx 2300\mu\text{m}$). Beyond this radius, charge is forced upwards

Figure 11. (a) The ring geometry and bias conditions resulting in the greatest active area and highest proportion of correctly-registered counts of the models tested thus far. Three 250 μm rings with 750 μm gaps. Equipotentials at 25V intervals. (b)-(e) Partition of charge collection between electrodes as a function of interaction position for the model (a). Active volume is represented by full anode charge collection. The sum of fractional charge collection by all electrodes at any location is 0 (black area) [Guard and Cathode not illustrated]. This 3D charge collection map is interpolated from Qrad profiles from simulated linescans at 12 depths. Figure 10 shows examples at the 3 depths indicated by white dashed lines.

and collected by the cathode (figure 10(a)). The lateral field at shallow depth is too weak to cause significant lateral drift.

At greater depths, anode charge collection extends further but charge is increasingly shared with Ring 1. At the radius where the bulk field switches polarity, the strong lateral field prevents charge from

drifting up to the cathode; instead, it is swept towards the axis until it experiences a bulk field component towards the anode face. Charge is forced diagonally downwards. Some reaches the anode; charge from deeper interactions at larger radii arrives at the anode face at the location of Ring 1, Ring 2 or Ring 3 and is captured.

If the guard were made less negative or removed, there would be no ‘cut-off’; the anode charge-sharing region in figure 11(b) would extend upwards to the cathode. These were the conditions that produced gradually-sloping Qrad profiles.

The problem of partial charge collection was not observed in experiment (figure 6). It is possible that the field conditions resulting from surface treatment and electrode deposition prevent charge from drifting too close to the surface and being captured by the rings. A more realistic model of the surface needs to be developed.

6. Conclusion

We have studied a 3-ring drift detector of 2.3mm-thick CZT by 25keV and 75keV microbeam scanning at room temperature. Voltages of all electrodes were independently varied to optimise performance. Our device displayed correct energy registration to the outer radius of its second ring. No peak ‘tailing’ was observed at 75keV, confirming that this is an effective single-carrier-sensing configuration. Resolution was limited by electronic noise. Our data show systematic trends in active area, peak position and sensitivity as lateral and bulk electric fields were varied. Future work will include experiments on similar devices with a noise-optimised electronic system.

The device was modelled in 3D with Sentaurus TCAD and linescans were simulated. Trends in performance with bias conditions were qualitatively reproduced but the model suffers from charge sharing between Ring 1 and the anode, which was not observed in experiment to this extent. Bias conditions of the model were optimised and found to be in the same ratio as the optimised experimental conditions.

Ring width, spacing, number and bias have been varied. Visualisation of charge drift, field conditions and multiple electrode signals have improved understanding of the parameters governing performance. In particular, the 3D shape of the active volume has been mapped and its relationship to bias and geometry is still under investigation. Narrowing the rings to the minimum size that can be fabricated has been shown to improve energy registration marginally. No 4-ring or 5-ring device has yet surpassed the performance of our best 3-ring design. Results suggest that the shape of the electric field on a wafer of this size and thickness is adequately controlled by 3 rings and cannot be further improved by extra steering electrodes.

Further changes in geometry will be investigated. Results of active volume mapping indicate that widening the first gap may increase charge collection for deep (high-energy) interactions. Charge sharing between the anode and rings must be eliminated in

order to reproduce experimental results accurately. A more realistic model of the field conditions at contact interfaces and gap surfaces is under development.

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Appendix A. Quality Factor of simulated ‘Qrad’ curves

The anode ‘Qrad’ curve (figure 5(c), *red*, figures 7,8(c)) shows the amount of charge collected by the anode when a single photon interacts at a certain radius in simulation. A Qrad curve is characteristic of a certain geometry, bias combination and interaction depth.

The simulation method used in this study does not generate spectra. The total effect of the complete and incomplete charge collection regions of the device is difficult to judge by inspection of their Qrad profiles. A quality factor was devised to quantify the relative performance of model devices.

It is supposed that the device is under uniform illumination of 1 photon per unit area at a single energy. All photons undergo photoelectric interaction.

The Qrad plot is normalised to a value of charge collected per count $Q = 1$ at the anode centre. Data points are interpolated by a piecewise cubic hermite interpolating polynomial (PCHIP) algorithm [36]. The region with $Q > 0.95$ charge collection is considered ‘flat-response’, radius r_{flat} , and its Q is rounded up to 1. Therefore the number of counts correctly registered is

$$1 \times \pi r_{\text{flat}}^2$$

The region of partial charge collection is divided into 250 bins with upper and lower relative charge collection limits Q_i and Q_j respectively. Radii at these limits are designated r_i and r_j . The number of counts in a bin is $1 \times$ the physical area of the annulus it represents.

The mean relative Q per interaction in the bin is approximately $(Q_i + Q_j)/2$. Thus a weighting factor $W = (1 - \frac{Q_i + Q_j}{2})$ is the difference between the charge collected per count in the bin and the correct value.

The ‘adverse impact’ of the bin upon spectrum quality is quantified as:

$$1 \times (\pi r_j^2 - \pi r_i^2) \times \left(1 - \frac{Q_i + Q_j}{2}\right)$$

Thus larger annuli with lower charge collection have a greater impact. The flat-response region has an impact factor of 0, by definition of W . The ‘impact factors’ of all annuli are summed from $r_i = r_{\text{flat}}$ up to the radius at which no charge is collected ($Q_j = 0$).

The overall ‘quality factor’ G of the (imagined) spectrum is defined as:

$$G = \frac{\pi r_{\text{flat}}^2}{\pi r_{\text{flat}}^2 + \sum \pi (r_j^2 - r_i^2) \left(1 - \frac{Q_i + Q_j}{2}\right)}$$

Thus the ideal spectrum has a quality factor $G = 1$ and a Qrad plot falling from $Q_i = 1$ to 0 at a single radius. Both the value of G and the active radius r_{flat} must be considered when judging the performance of a detector model.

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