Performance simulation and structure design of Binode CdZnTe gamma-ray detector Postprint

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Abstract

A new electrode structure CdZnTe (Cadmium Zinc Telluride) detector named Binode CdZnTe has been proposed in this paper. Together with the softwares of MAXWELL, GEANT4, and ROOT, the charge collection process and its gamma spectrum of the detector have been simulated and the detector structure has been optimized. In order to improve its performance further, Compton scattering effect correction has been used. The simulation results demonstrate that with refined design and Compton scattering effect correction, Binode CdZnTe detectors is capable of achieving 3.92% FWHM at 122 keV, and 1.27% FWHM at 662 keV. Compared with other single-polarity (electron-only) detector configurations, Binode CdZnTe detector offers a cost effective and simple structure alternative with comparable energy resolution.

Full Text

Preamble

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Performance Simulation and Structure Design of Binode CdZnTe Gamma-Ray Detector

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Abstract

This paper proposes a novel electrode structure for CdZnTe (Cadmium Zinc Telluride) detectors called the Binode CdZnTe detector. Using MAXWELL, GEANT4, and ROOT software, we simulated the charge collection process and gamma-ray spectrum of the detector and optimized its structure. To further improve performance, Compton scattering effect correction was applied. Simulation results demonstrate that with refined design and Compton scattering effect correction, Binode CdZnTe detectors can achieve 3.92% FWHM at 122 keV and 1.27% FWHM at 662 keV. Compared with other single-polarity (electron-only) detector configurations, the Binode CdZnTe detector offers a cost-effective and simple structural alternative with comparable energy resolution.

Keywords: Cadmium Zinc Telluride (CdZnTe), Binode CdZnTe detectors, Gamma-ray detector, Energy resolution
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Introduction

Benefiting from its high atomic number, high density, wide band gap, low chemical reactivity, and long-term stability, the semiconductor Cadmium Zinc Telluride (CdZnTe) radiation detector has been widely researched and applied in many fields including gamma-ray spectroscopy, X-ray imaging, and space physics [?, ?]. However, one major problem for CdZnTe detectors is low-energy tailing in the energy spectrum caused by hole trapping due to short carrier lifetime, crystal defects, and nonuniformity. To improve performance, many different single-polarity electrode structures have been proposed, including parallel strip Frisch grid [?], coplanar [?], CAPture [?], Quasi-hemisphere [?], and pixellated [?] designs.

With currently available high-quality crystals, CdZnTe detectors such as 3D depth-sensing position-sensitive (DSPS) devices [?] and coplanar grid detectors [?] achieve the best energy resolution. However, the readout electronics and integration costs of these devices are relatively high. 3D DSPS detectors always require more than 100 readout channels and complex computational overhead to perform depth and multiple-interaction corrections. Although Frisch ring and quasi-hemispherical devices require only a single readout channel and can be manufactured at lower cost, they typically achieve poor energy resolution and lower detection efficiency limited by their electrode structures.

In this paper, we propose a new electrode structure for CdZnTe detectors called Binode, which features two readout channels, and we have optimized the detector structure through simulation of the charge collection process and gamma-ray spectrum.

Detector Structure

A typical Binode CdZnTe detector is shown in Fig. 1 [Figure 1: see original paper]. The centers of both the upper and lower surfaces of the CdZnTe crystal are fabricated as anodes, while the four side surfaces form a single cathode. The main parameters of this detector are its physical dimensions (X, Y, Z), anode diameter (d), bias voltage (V), radiation incident direction, and electron and hole mobility-lifetime products (τ and τ), respectively. To achieve a symmetric electric field, the length and width of the crystal are typically equal (i.e., X = Y).

Performance Simulation

A. Simulation Process

In this study, we used software including MAXWELL, GEANT4, ROOT, and Induced Current Calculation (ICC, developed by our group to calculate induced current on semiconductor detector electrodes based on the Shockley-Ramo theorem). Fig. 2 [Figure 2: see original paper] shows the global simulation process. MAXWELL simulates the electrostatic field and weighting potential within the detector volume. GEANT4 is used to model the initial interaction and subsequent sub-interactions in the detector, tracking both the initial gamma rays and secondary particles created within the detector. The physics processes taken into account include photoelectric effect for gamma rays, multiple scattering and ionization for electrons, pair production, and Compton scattering. An energy threshold is typically set so that particles with kinetic energy below this limit are considered to have deposited their energy locally. In our simulation, thresholds of 20 keV for gamma rays and 5 keV for electrons were used. Once an interaction ends, the list of energy deposition points is transferred as a parameter to our charge transport code. ICC then calculates the carrier drift trajectories in the detector volume due to the electrostatic field and the induced current on the electrode, which depends on the weighting potential. The final calculated induced charges on the anodes are accumulated to generate the energy spectrum.

B. Electrostatic & Weighting Fields

Both the electrostatic and weighting fields within the detector volume critically affect charge collection performance. Based on the Shockley-Ramo theorem [**?**], the induced charge Q__{ind} is given by the weighting potential. The change in induced charge ΔQ__{ind} and the current i at an electrode caused by a charge q moving from x_i to x_j are given by:

ΔQ__{ind} = _{x_i}^{x_j} qE(x)dx, i = q E(x), where V(x) and E(x) are the weighting potential and field at position x. The total induced charge is actually the sum of charges induced by the drift of electrons and holes. The drift velocities and of free carriers through the detector volume depend on the electrostatic field, and the induced charge on the electrode is determined by the change in weighting potentials. For CdZnTe, the drift velocities are typically selected around 1400 $\mathrm{cm}^2/(\mathrm{s}\cdot\mathrm{V})$ for electrons and 120 $\mathrm{cm}^2/(\mathrm{s}\cdot\mathrm{V})$ for holes.

Applying a positive bias voltage to the anodes and 0 V to the side cathode, the electrostatic fields and weighting potentials were calculated by MAXWELL. Fig. 3(b) shows a mesh plot of a 2D slice (through the center of the anodes, shown in the left panel) of the electric potential when 800 V bias is applied. It is immediately clear from Fig. 3 that due to the fact that the four sides of the cathode are at the same potential, the binode electrode geometry reduces the electric potential throughout the detector volume compared to a planar detector. Fig. 4(a) shows a mesh plot of a 2D slice of the weighting potential of anode I, and Fig. 4(b) shows the weighting potential of anode II. The slice shown is also indicated in Fig. 3(a). Although the reduced electric field strength will locally slow free carriers down and increase trapping probabilities, the benefit of the binode design is greatly improved charge collection due to suppression of the weighting potential as seen in Fig. 4. To achieve significant improvement in charge collection, one must accept the reduced electric field strength in the Binode design.

To understand the free carrier drift more closely, we selected several positions in the detector volume to track electron trajectories. Fig. 5 gives the calculation results (the detector volume is 10 mm × 10 mm × 5 mm), where the x-coordinate of the selected points is 0 mm, y-coordinates range between -5 mm and 5 mm (interval 1 mm), and z-coordinates are 2.4 mm and 2.6 mm. For hole trajectories in the detector volume, one can simply exchange the start and end points of electrons, as holes drift in the opposite direction of electrons.

C. Correction of the Compton Scattering Effect (CCSE)

Obviously, when carriers drift in the detector volume, both anodes will receive signals. For a photoelectric effect event, the free carriers will induce a positive signal on the anode where electrons are finally collected, while a negative signal will be induced on the other anode. The positive signal will be larger than the negative one because the weighting potential of the collecting anode accumulates more charge than the other anode along the carrier motion path. In this case, we add the absolute values of both anode signals together as the final induced charge. However, for Compton scattering or pair production events where carriers are created separately in both the upper and lower detector volumes, the created carriers will be collected by both anodes, resulting in two positive signals observed on both anodes. In this case, we add both positive signals together to obtain the final induced charge.

Figure 6 [Figure 6: see original paper] shows the scatter diagram of induced charge on the two separated anodes, where positive induced charge means electron collection, while negative induced charge occurs without electron collection on the anode electrode. However, for those Compton scattering and pair production events mentioned above where created electrons are collected by different anodes, both anodes will be induced with positive charge, as shown in area (a). Area (b) shows twice Compton scattering without complete energy deposition, and area (c) shows photoelectric effect events and single Compton scattering events.

The results show that after CCSE, the performance of the Binode CdZnTe detector improved significantly. Fig. 7 [Figure 7: see original paper] shows the simulated energy spectrum before and after CCSE. Due to CCSE, the FWHM of the ^{137}Cs 662 keV gamma-ray spectrum improved from 3.31% to 1.27%, and the peak-to-Compton ratio increased from 2.4 to 7.4. Fig. 8 [Figure 8: see original paper] shows the simulation results of ^{137}Cs 662 keV and ^{57}Co 122 keV gamma-ray spectra with CCSE, where the detector dimensions are X=Y=Z=10 mm, bias voltage is 3000 V, and the pixel anode diameter D=3 mm. This CdZnTe detector with CCSE achieved 3.92% FWHM at 122 keV and 1.27% FWHM at 662 keV without electronic noise.

Parameters Optimization

A. Length-to-Thickness Ratios (X/Z)

We simulated two detector structures with different length-to-thickness ratios (X/Z = 1 or 2), with results shown in Fig. 9 [Figure 9: see original paper]; both included CCSE. The simulation results demonstrate that when X/Z = 1, the detector exhibits better performance, meaning the detector has equal dimensions (X=Y=Z).

B. Anode Size and Bias Voltage

The left panel of Fig. 10(a) [Figure 10: see original paper] shows the spectral performance for a 10 mm × 10 mm × 10 mm Binode CdZnTe detector with anode diameters between 1 mm and 4 mm. The results show that when D = 3 mm, the detector achieves excellent performance with energy resolution of about 1.28% FWHM at 662 keV when 3000 V is applied to both anodes. The right panel of Fig. 10(a) shows the simulated ^{137}Cs spectral response of a 10 mm × 10 mm × 10 mm Binode CdZnTe detector with D=3 mm pixel anodes at bias voltages between 2800 V and 3200 V. The CdZnTe crystal was chosen to have low electron transport with $\tau = 7 \times 10^{-3}$ cm^2/V and hole transport with $\tau = 3 \times 10^{-5}$ cm^2/V.

The simulation results demonstrate that the anode diameter D should not be too small, as shown in Fig. 10(a) (left) with D = 1 mm. The poor spectral performance is mainly due to the weak electric field caused by the small anode diameter. However, with D = 4 mm, the spectrum also becomes worse, primarily because the pixelated effect is not pronounced due to the larger anode diameter. The left panels of Fig. 10(b) and Fig. 10(c) show the simulation results of spectral performance for 5 mm × 5 mm × 5 mm and 15 mm × 15 mm × 15 mm Binode CdZnTe detectors with varying anode sizes. The results indicate that the optimal ratio of anode size to detector thickness is about 0.2–0.3, i.e., D/Z = 0.2–0.3.

The simulation results for Binode CdZnTe detectors with varying anode voltages are also shown in Fig. 10 (right), demonstrating that the anode voltage relative to detector thickness should be rationally designed at about V/Z = 250–300 V/mm.

Based on the above results, for a 5 mm × 5 mm × 5 mm Binode CdZnTe detector, the best energy resolution was about 1.24% with an anode diameter of 1.5 mm and voltage of 1400 V. The best energy resolutions for 10 mm × 10 mm × 10 mm and 15 mm × 15 mm × 15 mm Binode CdZnTe detectors are 1.27% and 1.78% at D = 1.5 mm, V = 2800 V and D = 2.25 mm, V = 3500 V, respectively.

Conclusion

In this study, we proposed a novel electrode structure for CdZnTe detectors called the Binode CdZnTe detector. Based on simulations, we numerically investigated the dependence of Binode CdZnTe detector performance on design parameters such as length-to-thickness ratios, anode pixel diameter, and bias voltage (i.e., X/Z, D, and V). The results show that with optimized design and Compton scattering effect correction, the Binode CdZnTe detector can achieve excellent performance. The simulation data can also be used to develop design criteria for Binode CdZnTe detectors to improve test yields and thereby reduce manufacturing costs.

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