TCAD simulation of a proposed 3D CdZnTe detector

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Abstract: Cadmium zinc telluride (CdZnTe) detectors are potential replacements for traditional room temperature detectors, such as silicon (Si), in many applications. CdZnTe has been considered as a promising semiconductor material for hard X-ray and Γ-ray detection because the stopping power of CdZnTe is better than traditional materials. To exploit them for practical applications, their behaviour under harsh conditions must be fully characterised and understood. In this study, the electrical characteristics of the CdZnTe three-dimensional (3D) detector are comprehensively studied through TCAD simulations. The very low leakage current, which is about 5.5 pA at 200 V, allows applying higher bias voltages than possible with traditional two-dimensional (2D) detectors. Moreover, the effect of the temperature on the leakage current is studied. Additionally, the collection time is found to be about 2 ns and the amplitude of the current is 0.8 nA at 200 V. The obtained results prove the applicability of the CdZnTe 3D detector under various operating conditions.

1 Introduction

In recent years, extensive work has been devoted to developing a range of compound semiconductors with a wide band gap and high atomic number for radiation detectors [1]. Cadmium telluride (CdTe), zinc telluride (ZnTe) and cadmium zinc telluride (CdZnTe) are the most semiconductor materials that have obtained significant attention as X-ray and Γ-ray detectors because of their low leakage current and high detection efficiency at room temperature [2]. These compounds have a lot of applications including optoelectronics, microelectronics, sensor electronics and photovoltaics [3–5].

Radiation detectors using CdZnTe may operate at room temperature, so, it is different from some other materials that need the liquid nitrogen cooling system [6]. Although silicon (Si) and germanium (Ge) have superb charge-transport and energy resolution, they have low stopping power for high energy photons. This limits their application, as detectors, to hard X-ray and Γ-ray detection. Furthermore, Ge detectors must operate at cryogenic temperatures as Ge has a small band gap [6]. In contrast, CdZnTe detectors have energy resolution close to high-purity germanium.

Due to the high resistivity of CdZnTe, higher atomic binding energy and the ability to vary the band gap of the material in the range from $E_g = 1.46$ eV (CdTe) to $E_g = 2.26$ eV (ZnTe), CdZnTe has many advantages over CdTe in the development of high efficiency X-ray and Γ-ray detectors [7, 8]. Furthermore, the increased band gap of the detector materials results in reduced leakage current. Also, the strong bonding between Zn and Te allows high detection efficiencies [6]. The best spectral behaviour is attained with a zinc fraction of about 10%, so it can work at a lower voltage than CdTe [9].

In this study, the electrical characteristics of the three-dimensional (3D) detector are studied through TCAD simulations. TCAD simulations are considered as a powerful tool to examine new detector structures before fabrication [10]. The results of the *I–V* characteristic, *C–V*, and output current are obtained at 100 V, 200 V at 75 keV energy of the incident beam. Furthermore, the effect of temperature on the leakage current is demonstrated at 21.5 and 70°C.

2 Device calibration

In this section, we calibrate the simulation parameters versus measurements carried out in [11]. This calibration is performed to confirm that the parameters used in simulations are practicable for CdZnTe device simulations. The calibrated device is a CdZnTe two-dimensional (2D) detector grown by the high pressure Bridgman technique. The volume of the detector is $4 \times 4 \times 2\ \text{mm}^3$ and measurements of the leakage current are performed at 20°C. In the simulation, all physical parameters, like mobility and energy gap, are taken temperature-dependent. The leakage current of the measured structure and our simulation are compared in Fig. 1 showing good agreement. The calibrated parameters are: $\mu_e \tau_e = 6.07 \times 10^{-3}\ \text{cm}^2/\text{V}$ and $\mu_h \tau_h = 8.82 \times 10^{-4}\ \text{cm}^2/\text{V}$, where $\mu\tau$ is the mobility-lifetime product.

3 Design of the 3D CdZnTe detector

Firstly, the 3D detector structure is designed with a p-type substrate. The specific details of the simulated structure are as follows. The p-type substrate is 300 µm thick, with $7 \times 10^{11}\ \text{cm}^{-3}$ acceptor doping concentration. The columns are cylindrical with 5 µm in radius and consist of doped CdZnTe. The n- and p-type columns have $6 \times 10^{10}\ \text{cm}^{-3}$ donor- and acceptor-doping concentration, respectively, as shown in Fig. 2. This substrate thickness is chosen to be compatible with the thickness of certain ATLAS 3D sensors [12]. For the simulations presented in this work, a pixel size of 55 µm was chosen, so the simulation structure has a volume of 55 µm × 55 µm by 300 µm. This is a relatively small pixel size, corresponding to the Medipix2 readout chip [13].

In the full 3D detector shown in Fig. 2*a*, the electrode columns pass through the full thickness of the substrate and are connected on the front surface. Each cell consists of one central p-type electrode that is 10 µm in diameter and surrounded by four similar n-type electrodes in a square array with 10 µm in diameter. The top surface is covered by SiO_2 with 1 µm thickness and the contacts are made of aluminium above the electrodes with a diameter of 8 and 2 µm thickness. A 2D horizontal cross-section of the doping concentration distribution is shown in Fig. 2*b*.

In the following 3D TCAD simulations, all important physical parameters are enabled. The electron and hole mobility lifetime products are taken as the calibrated values. The other physical parameters, like mobility and energy gap, are taken as functions of temperature.

4 Simulation results

In this section, simulation results are presented. Firstly, the leakage current and temperature effect on it are shown. Then, the transient

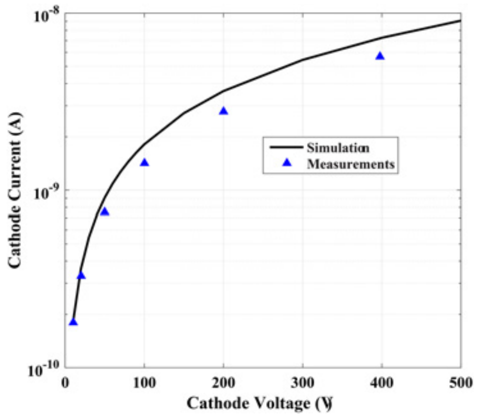

Fig. 1 *Calibration of simulation versus measurements of 2D detector structure*

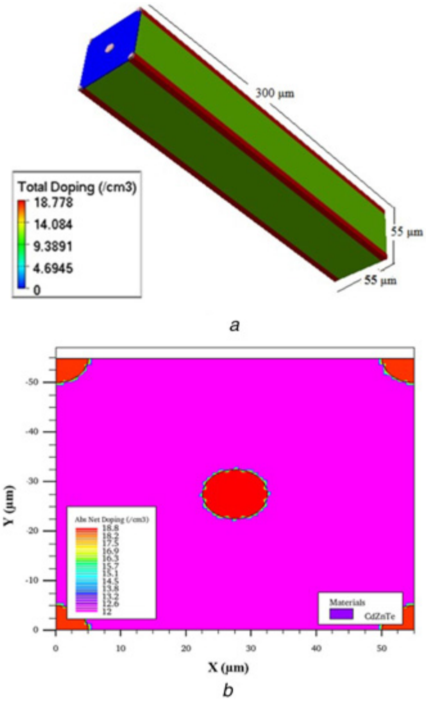

Fig. 2 *Basic structure used in simulation using SILVACO*
a 3D view
b Doping concentration in a horizontal cross-section

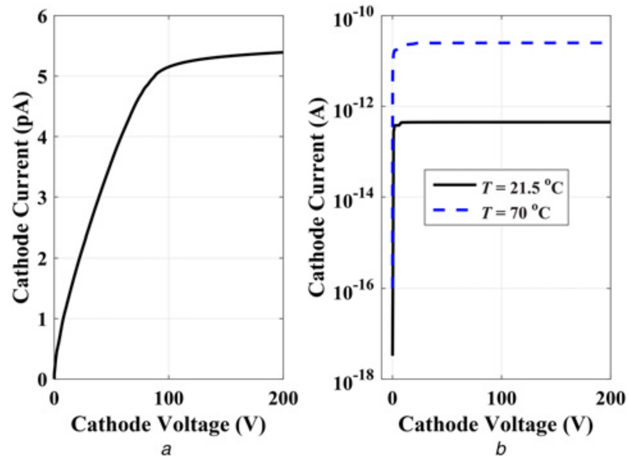

Fig. 3 *Leakage current at*
a Room temperature
b Two different temperatures

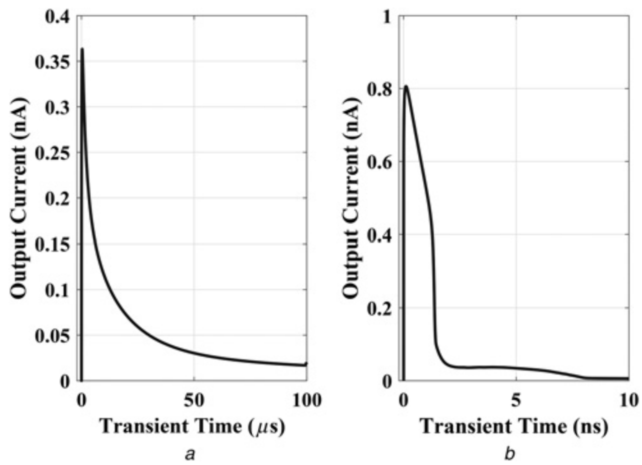

Fig. 4 *Output current at*
a Voltage of 100 V and 75 keV
b Voltage of 200 V and 75 keV

simulation of the output current is presented. Finally, the small signal analysis is shown in terms of capacitance.

The leakage current of a detector based on a reverse-biased junction depends directly on the generation–recombination lifetime τ which, in turn, depends strongly on the concentration of states close to the mid-gap. After irradiation, the increased concentration of defects leads to an increase of the leakage current. It has been demonstrated that the increase of the leakage current after irradiation of fast hadrons is proportional to the fluency [14] and does not depend on the material. The high-electrical resistivity reduces the leakage current to values compatible with the low noise electronics used to process the individual pulses. The energy resolution of the detector is a strong function of leakage current and noise. Fig. 3*a* shows the leakage current of the 3D detector at room temperature.

Although the CdZnTe detector is a candidate for room temperature operation, its performance depends on the temperature variations. If a high-resolution X-ray or Γ-ray spectroscopy system with a CdZnTe detector is to be made, the effect of the temperature on the CdZnTe detector should be understood. The detector's performance must be stable with varying temperature. In Fig. 3*b*, the leakage current is increased with temperature, as expected, from 21.5 to 70°C as indicated.

The transient simulation is used to investigate the charge collection behaviour in the proposed 3D detector at different voltages. The simulation is done by flooding the device with a uniform concentration of electron–hole pairs (75e–h pairs/µm) at 100 V as shown in Fig. 4*a*. The charge collection time is a strong function of bias voltage. As the voltage increases, the collection time decreases. At a bias voltage of 100 V, the collection time is 6×10^{-5} s and at 200 V the collection time is 2×10^{-9} s as shown in Fig. 4*b*.

Finally, the 3D detector structure is simulated to calculate the capacitance between the n^+ bias columns and p^+ readout columns at a frequency of 1 MHz and a bias of 200 V. Fig. 5 shows the total readout capacitance seen at each pixel. The capacitance decreases with increasing the bias voltage as the space charge region width increases. A minimum value of 40 fF is achieved at $V_k \geq 20$ V. It is obvious that the capacitance in the 3D detector structure is greater than that of the planar detector.

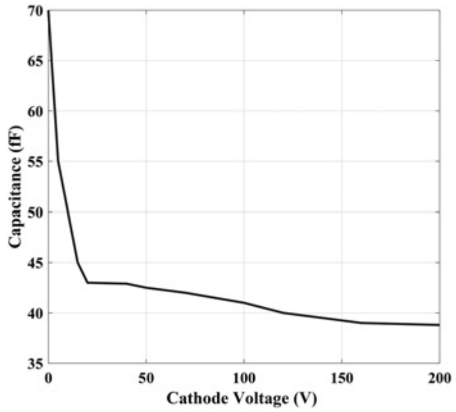

Fig. 5 *Capacitance versus voltage characteristics of the CdZnTe 3D detector*

It is worth mentioning that the leakage current of the proposed CdZnTe 3D detector is 0.1 pA at 3.3 V, while the leakage current of Si detectors [10], for the same shape and design, is 9 nA at the same voltage. This is due to the large gap of CdZnTe compared with Si. Moreover, the capacitance of the Si detector is 0.3 pF at 10 V while it is 50 fF for CdZnTe at the same voltage because of the low intrinsic carrier of CdZnTe. Although the output current of the CdZnTe detector is less than that of Si, the ratio of the output to leakage current is acceptable.

5 Conclusions

The 3D CdZnTe detector has been simulated using SILVACO TCAD. To design the detector, a substrate thickness of 300 µm is used to meet the new technology of hardness radiation. The leakage current is found to be about 5.5 pA at room temperature under 200 V reverse bias, which is a subtle value relative to the planar cell. Additionally, the temperature effect on the 3D detector's leakage current is studied. The *I–V* and *C–V* characteristics and output current under transient simulations are obtained and presented. We conclude that the proposed design of such a detector provides a fast charge collection that meets the radiation hardness requirements. This work paves a light that CdZnTe could be regarded as a potential candidate for the next generation of X-ray and hard Γ-ray detectors.

6 References

[1] Del Sordo S., Abbene L., Caroli E., ET AL.: 'Progress in the development of CdTe and CdZnTe semiconductor radiation detectors for astrophysical and medical applications', *Sensors*, 2009, **9**, (5), pp. 3491–3526

[2] Xu H., Xu R., Huang J., ET AL.: 'The dependence of Zn content on thermal treatments for $Cd_{1-x}Zn_xTe$ thin films deposited by close-spaced sublimation', *Appl. Surf. Sci.*, 2014, **305**, pp. 477–480

[3] Triboulet R., Siffert P. (Eds.): 'CdTe and related compounds; physics, defects, hetero- and nano-structures, crystal growth, surfaces and applications (European Materials Research Society Series)' (Elsevier, Amsterdam, The Netherland, 2009, 1st edn.)

[4] Wu Y.L., Chen Y.T., Feng Z.C., ET AL.: 'Synchrotron radiation x-ray absorption fine-structure and Raman studies on CdZnTe ternary alloys'. SPIE Optical Engineering and Applications, August 2009, p. 74490Q

[5] Yang G., Kim D., Kim J.: 'Photosensitive cadmium telluride thin-film field-effect transistors', *Opt. Express*, 2016, **24**, pp. 3607–3612

[6] Eisen Y., Shor A.: 'Cdte and CdZnTe materials for room-temperature X-ray and gamma ray detectors', *J. Cryst. Growth*, 1998, **184**, (185), pp. 1302–1312

[7] Stolyarova S., Edelman F., Chack A., ET AL.: 'Structure of CdZnTe films on glass', *J. Phys. D: Appl. Phys.*, 2008, **41**, (6), p. 065402

[8] Abbene L., Gerardi G., Turturici A.A., ET AL.: 'X-ray response of CdZnTe detectors grown by the vertical Bridgman technique: energy temperature and high flux effects', *Nucl. Instrum. Methods Phys. Res. A, Accel. Spectrom. Detect. Assoc. Equip.*, 2016, **835**, pp. 1–12

[9] James R.B., Schlesinger T.E., Lund J., ET AL.: '$Cd_{1-x}Zn_xTe$ spectrometers for gamma and X-ray applications', *Semicond. Semimet.*, 1995, **43**, pp. 335–381

[10] Abouelatta M., Shaker A., Gontrand C., ET AL.: 'Performance of standard and double-sided 3D-radiation detectors under the impact of a temperature pulse', *IET Electron. Lett.*, 2015, **51**, (21), pp. 1668–1670

[11] Takahashi T., Watanabe S.: 'Recent progress in CdTe and CdZnTe detectors', *IEEE Trans. Nucl. Sci.*, 2001, **48**, (4), pp. 950–959

[12] Wright V.A., Blue A., Horn M., ET AL.: '3D detectors-a new direction for Medipix', *Nucl. Instrum. Methods Phys. Res. A, Accel. Spectrom. Detect. Assoc. Equip.*, 2004, **531**, (1), pp. 56–61

[13] Wright V.A., Davidson W.D., Melone J.J., ET AL.: 'Three-dimensional Medipix – a new generation of X-ray detectors', *IEEE Trans. Nucl. Sci.*, 2005, **52**, (5), pp. 1873–1876

[14] Schlesinger T.E., Toney J.E., Yoon H., ET AL.: 'Cadmium zinc telluride and its use as a nuclear radiation material', *Mater. Sci. Eng. R*, 2001, **32**, (4), pp. 103–189