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Simulation of active-edge pixelated CdTe radiation detectors

D.D. Duarte [a,b,*], J.D. Lipp [a], A. Schneider [a], P. Seller [a], M.C. Veale [a], M.D. Wilson [a], M.A. Baker [b], P.J. Sellin [b]

[a] STFC Rutherford Appleton Laboratory, Harwell Oxford, Didcot OX11 0QX, United Kingdom
[b] Faculty of Engineering and Physical Sciences, University of Surrey, Guildford, Surrey GU2 7XH, United Kingdom

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ABSTRACT

The edge surfaces of single crystal CdTe play an important role in the electronic properties and performance of this material as an X-ray and γ-ray radiation detector. Edge effects have previously been reported to reduce the spectroscopic performance of the edge pixels in pixelated CdTe radiation detectors without guard bands. A novel Technology Computer Aided Design (TCAD) model based on experimental data has been developed to investigate these effects. The results presented in this paper show how localized low resistivity surfaces modify the internal electric field of CdTe creating potential wells. These result in a reduction of charge collection efficiency of the edge pixels, which compares well with experimental data.

1. Introduction

Cd(Zn)Te single module devices have shown encouraging results for X-ray imaging but many applications, such as nuclear medicine and airport security, require larger radiation detectors. Large area Cd(Zn)Te crystals are limited to the maximum ingot sizes of 85 mm in diameter and pixelated devices are restrained to the reticle size of the ASIC used in the foundry (typically $<2\times 2\ \mathrm{cm}^2$). Cd(Zn)Te modules can be tiled together to form a larger detector array [1–3]. This structure produces gaps between modules due to the space taken by the ASIC readout and by the guard band in the sensor and can be detrimental for X-ray imaging, particularly in medical applications. Through Silicon Via technology and active-edge detectors, where pixels are sensitive up to the physical edge of the device, are required to minimize these gaps and build a large panel Cd(Zn)Te detectors for X-ray imaging.

Guard bands have been employed in radiation detectors since the 1960s to mitigate edge effects due to the presence of defects in the physical edge of the CdTe detector created by wafer dicing without subsequent edge treatment. Many studies have investigated the effect of the surface preparation of Cd(Zn)Te prior to the deposition of contacts where reductions in leakage currents in Cd(Zn)Te radiation detectors and better adhesion and electrical properties of the electrical contacts deposited are achieved [4–8]. However, little has been done to investigate the effect of edge processing in Cd(Zn)Te radiation detectors. J. Crocco et al. have reported that mechanical polishing of the edge decreases detector leakage currents by 200% when a surface rms roughness of 20 nm is achieved [9], but the 1 mm thick CdTe radiation detectors supplied by Acrorad rely on a smooth wafer dicing process to decrease edge damage and subsequent leakage current.

The STFC Rutherford Appleton Laboratory has developed a pixelated active-edge Acrorad CdTe radiation detector bonded to the HEXITEC ASIC. HEXITEC is a fully spectroscopic readout ASIC for X-ray imaging up to 200 keV that is able to read the position and energy of each interacting photon [10]. The active-edge detector configuration has a 250 μm pixel pitch where the guard band has been removed and the edge pixels extended to the physical edge of the crystal. Non-uniformities in the spectroscopic performance of this HEXITEC active –edge CdTe detector with Acrorad diced edges were present in only 13% of the edge pixels and these were typically characterized by a reduction in the charge collection efficiency [11].A study with a 10 μm × 10 μm 20 keV monochromatic beam at the Diamond Light Source synchrotron showed that in these pixels a non-uniform reduction in the electric field up to 200 μm from the crystal edge in these pixels was responsible for the poor performance [11]. These promising results show that the majority of edge pixels have excellent spectroscopic performance in detectors with Acrorad diced edges, but that the spatial variation in non-uniformities at the crystal edges need to be further understood.

* Corresponding author at: STFC Rutherford Appleton Laboratory, Harwell Oxford, Didcot OX11 0QX, United Kingdom. Tel.: +44 1235 44 5195.
E-mail address: diana.duarte@stfc.ac.uk (D.D. Duarte).

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The edge leakage current of these devices has been measured to be at least an order of magnitude higher than the bulk leakage current [11] which suggests the presence of low surface resistivity at the edge of CdTe. Nevertheless, it is difficult to find a method to experimentally measure and understand the edge resistivity of thick semi-insulating samples created by dicing or edge processing and its subsequent effect on the electric field near the crystal edge.

This difficulty is addressed in here by using TCAD simulation models to understand the surface properties of CdTe and to replicate effects observed experimentally in these detectors. This will allow the development of processes to minimize edge effects and to increase the active area as the industry moves forward to commercialize large panel Cd(Zn)Te radiation detectors.

2. The TCAD simulation software

TCAD is a finite-element simulation package developed by Synopsys® [12] for the silicon industry to optimize semiconductor processing technologies and devices. It is possible to design and simulate the electric characteristics of semiconductor radiation detectors using tools such as the Structure Editor and Sentaurus Device. TCAD can also be used to simulate other materials than silicon, such as CdTe, but the number of TCAD models and tools applicable to these materials is restricted.

The CdTe device is created in the TCAD software using geometric operations that define the bulk crystal and electrodes in either 2D or 3D. In this paper, only 2D structures were simulated. The device structure is modeled using a finite element discretization by creating a 2D mesh of nodes and fragmenting the volume between the nodes into several elements. The semiconductor equations are approximately defined for each element during simulation where the three main variables are the electron and hole concentrations and the electrostatic potential [13]. The primary focus of the semiconductor equations in simulation is to describe the static and dynamic behavior of charge carriers under the influence of electrical fields [14]. The motion of charge carriers is treated to be semi-classical hence the transport of electron and holes in semiconductors is derived from the Boltzmann transport equations. It is incorporated in TCAD through the drift-diffusion model, where the current densities, $\vec{J}_{n,p}$, for electrons and holes are given by (1) and (2) respectively:

$$\vec{J}_n = -nq\mu_n \nabla\varphi_n \tag{1}$$

$$\vec{J}_p = -pq\mu_p \nabla\varphi_p \tag{2}$$

where n and p the electron and hole carrier densities, $\mu_{n,p}$ the electron and hole mobility and $\nabla\varphi_{n,p}$ the gradient of $\varphi_{n,p}$, which are the electrostatic potential (or quasi-Fermi potentials) due to electrons and holes.

All of the carrier transport models for semiconductors can be written in the form of the continuity equations that describe charge conservation, given by (3) for electrons and (4) for holes:

$$\nabla J_n = qR + q\frac{d_n}{d_t} \tag{3}$$

$$-\nabla J_p = qR + q\frac{d_p}{d_t} \tag{4}$$

where R is the net recombination rate and q the electron electric charge.

2.1. Boundary conditions

The solutions to the semiconductor equations require boundary conditions for the contact surfaces and other borders, such as the device edges. Ohmic contacts are used in this simulation for simplicity where charge neutrality and equilibrium and zero barrier height at the metal–semiconductor interface are assumed. The ideal Neumann boundary conditions, also known as reflective boundaries, are adopted at the device edges as artificial boundaries to guarantee that the domain under consideration is self-contained. These state that no current flow exists at the interface, according to (5) for electrons and (6) for holes:

$$J_n . n = 0 \tag{5}$$

$$J_p . p = 0 \tag{6}$$

The boundary conditions adopted are particularly important when simulating active-edge devices or the effect of guard bands on the electric performance of any radiation detector.

2.2. Simulation parameters

In this paper, a simulation model that reflects edge effects will be validated against experimental data previously published by Duarte et al. [11]. CdTe detectors were investigated using 20 keV monoenergetic X-ray photons. These create a charge cloud 79.73 μm below the detector cathode corresponding to the mean free path of 20 keV photons in CdTe, calculated using the NIST XCOM software [15]. The charge generated by 20 keV is equivalent to 7.22×10^{-4} pC. A *w-value* of 4.43 eV per electron-hole-pair was used for this calculation [16].

A 1 mm thick device made from the standard CdTe material in the TCAD library was used in the simulation. No trap states are present in this material and the charge carrier mobilities (μ) and lifetimes (τ) have values of: $\tau_e = 5$ μs, $\tau_h = 0.5$ μs, $\mu_e = 1000$ cm^2(V s)$^{-1}$, $\mu_p = 80$ cm^2.(V s)$^{-1}$. The charge collecting time implemented in the simulation is of 2 μs, the same value as the shaping time used in the HEXITEC ASIC, in order to compare experimental data with simulation data.

This device was biased at -400 V. It is defect-free (no traps or dopants present) and has a bulk resistivity of 6.9×10^{10} Ω cm, an order of magnitude higher than commercial available CdTe ($\sim 10^9$ Ω cm) [17]. To build an ideal CdTe material in TCAD would require knowledge of the doping and trapping states in the material that are beyond the purpose of the simulations presented here. Hence, all the resistivity values used in this simulation are relative to the bulk resistivity of the TCAD material.

3. TCAD simulation of a pixelated CdTe

The most important parameters in a semiconductor radiation detector simulation are the electric field, electrostatic potential and weighting potential that determine the path the charge carriers will follow and the charge induced in a pixel. Fig. 1a) shows the electric field profile for an active-edge pixelated CdTe detector with a 250 μm pixel pitch and an edge pixel of 350 μm.

The electric field strength is uniform throughout the bulk of the detector but shows an increase in field strength closer to the pixel contacts with a decrease of field between pixels. Fig. 1b) shows the electrostatic potential for the same device where charge carriers travel perpendicularly to the equipotential lines.

Another parameter of interest is the pixel weighting potential which is solely reliant on the detector geometry. The weighting potential is a theoretical tool that is used to describe charge induction in small pixel detectors [18]. In an imaging geometry, the weighting potential near the anode can be enhanced by reducing the pixel size relative to the thickness of the detector. This phenomenon is known as the “small pixel effect” and ensures that only charge carriers that drift close to the detector pixels induce a significant charge. This is important in CdTe detectors where the poor transport of holes can

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