Simulation Studies of CdTe Pixel Detectors

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***Abstract*–We have performed simulation studies of CdTe pixel detectors using the commercial SDEVICE simulator by SYNOPSYS. We have incorporated energy levels and concentrations of defects in the band gap using the information by published compensation models. We have performed I-V simulation experiments. We simulated the transient behavior of the detectors due to the bombardment with alpha particles and X-ray photons. The simulation of the interaction with alpha particles required the description of the dependency on energy of the Bragg peak in CdTe, which we included in the material database file of CdTe. We investigated the relation of the charge collected at neighbor pixels with the depth of interaction of X ray quanta. The study has the following purposes: (a) To provide realistic current waveforms as input to electronics simulations needed for the development of pixel readout electronics. (b) To evaluate methods for the extraction of the depth of interaction. (c) To incorporate to this device simulator as much detailed information as possible about the material, about the electrodes and about the defects that degrade its performance and explore through numerical simulation their effect on charge collection.**

I. Introduction

THE detailed and accurate modeling of CdTe detectors is a demanding task due to the lack of consistent information about various material parameters, as well as the fact that the compensation mechanism details have not been clarified yet.

In this study we used the commercial device simulator SDEVICE[1] by SYNOPSYS. The equations which we solved were:

The Poisson equation

$$\nabla \cdot \varepsilon \nabla \varphi = -q(p - n + N_D - N_A) - \rho_{TRAP}$$

coupled with the electron continuity equation

$$\nabla \cdot \left(-nq\mu_n \nabla \Phi_n\right) = q(R_{net} + \frac{\partial n}{\partial t})$$

and with the hole continuity equation

$$\nabla \cdot \left(-pq\mu_p \nabla \Phi_p\right) = q(R_{net} + \frac{\partial p}{\partial t})$$

Where φ is the electrostatic potential computed as the difference from a reference potential which is the Fermi potential of the intrinsic material, Φ_n and Φ_p are the quasi-Fermi potentials for electrons and holes respectively, R_{net} is the net electron – hole recombination rate, N_D and N_A are the ionized donor and acceptor concentrations, ρ_{TRAP} is the charge density contributed by traps and fixed charges.

The values of the main parameters used are collected in Table 1:

TABLE I
MATERIAL PARAMETERS

Parameter	Value
ε_r relative permittivity of CdTe	10.6
Bandgap (@300^{o}K)	1.52
Electron effective mass	0.096
Hole effective mass	0.43
Electron affinity	4.28eV
Electron mobility (@300^{o}K)	1000cm^2/V·s
Hole mobility (@300^{o}K)	80cm^2/V·s

The first objective of our study was to create a model for the material consistent with well established experimental results. This would make us confident about the results of the charge transport simulations, which was our second objective. The information contained in the materials database of the simulator is elementary. The material is described as a pure homogeneous crystal without any defects, while some parameters have default values, which are wrong, because they are borrowed from Silicon. One example is the Brag peak position used in the generation term of the continuity equations when the charge deposition from an alpha particle is simulated. We used the SRIM package [2] to simulate the spectra of the energy deposited by alpha particles with different energies impinging on CdTe. Then we extracted the parameters of the fit of a second order polynomial which relates the position of the Brag peak to the energy of the alpha particle and used it in the generation term (see [1] pp 431-432):

$$G(u,v,w,t) = \left(k/(2\pi)^{1/2} \cdot s\right) \cdot$$
$$\exp\left(-\frac{1}{2}\right)\left[\frac{(t-t_m)^2}{s^2} + \frac{v^2+w^2}{w_t^2}\right]\left[c_1 e^{au} + c_2 \exp - \frac{1}{2} \cdot \left(\frac{u-a_1}{a_2}\right)^2\right]$$

if $u \le a_1 + a_3$, else $G(u,v,w,t) = 0$

Where u is the coordinate along the alpha particle path, v and w are the coordinates orthogonal to u, α_1 is the position of the Brag peak obtained from the relation: $a_1 = b_0 + b_1 E + b_2 E^2$. The scaling factor k is obtained from the constraint that the integral of the generation term over space and time is equal to

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E/E_P where E is the energy of the alpha and E_P is the mean electron – hole creation energy. The parameter c_1 is given by the relation: $c_1 = \exp[\alpha \cdot (a_1(10MeV) - a_1(E))]$

The parameter values used are given in Table 2, where in bold are the non default ones.

TABLE 2
PARAMETERS USED IN THE GENERATION TERM FOR ALPHA PARTICLES

B_0	**$-2.052 \cdot 10^{-4}$ cm**
B_1	**$2.665 \cdot 10^{-10}$ cm/eV**
B_2	**$2.549 \cdot 10^{-17}$ cm/eV^2**
E_P	**4.43 eV**
S	$2 \cdot 10^{-12}$ sec
w_t	$1 \cdot 10^{-5}$ cm
A	90 cm^{-1}
A_2	$5.5 \cdot 10^{-4}$ cm
A_3	$2 \cdot 10^{-4}$ cm

II. MODELLING OF THE SEMI-INSULATING MATERIAL

Since the default material description does not include donors, acceptors and traps, we introduced two well known compensation models [3],[4] to obtain semi-insulating material.

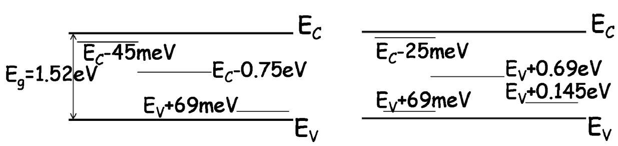

Fig. 1. Energy levels in the band gap of doping, complexes and deep level traps in accordance with the two compensation mechanism models included in the material description.

The parameters we used are collected in the Table 3:

TABLE 3

Electron and hole capture cross section	10^{-15} cm^2
Concentrations in cm^{-3}	
Model of [3]	Model of [4]
$5 \cdot 10^{16}$ @E_C – 45 meV	$5.017 \cdot 10^{16}$ @E_C – 25meV
$6 \cdot 10^{16}$ @E_V + 69 meV	10^{14} @E_V + 69 meV
	$4.983 \cdot 10^{16}$ @E_V + 0.145 eV

The dependence of the resistivity on the concentration of the deep levels is plotted in Fig. 2 and 3 for the two models. Resistivity of the order of $10^9 - 10^{10}\Omega \cdot cm$ is obtained with deep level concentrations of the order of 10^{16} for the model of [3] and of $2 \cdot 10^{14}$ for the model of [4].

The one of the contacts of a high resistivity crystal was defined as Schottky type and the Indium work-function (4.21eV) was used. The result of the calculation of the electric field profile for the concentration of the deep level that made the material highly resistive is given in Fig. 4. It turns out that the electric field is close to zero in most of the volume of the detector and that it increases abruptly in a thin layer close to the positively biased electrode. Moreover the increase of bias has little effect in the increase of the depletion region. This result means that most of the volume of the detector is not sensitive to radiation.

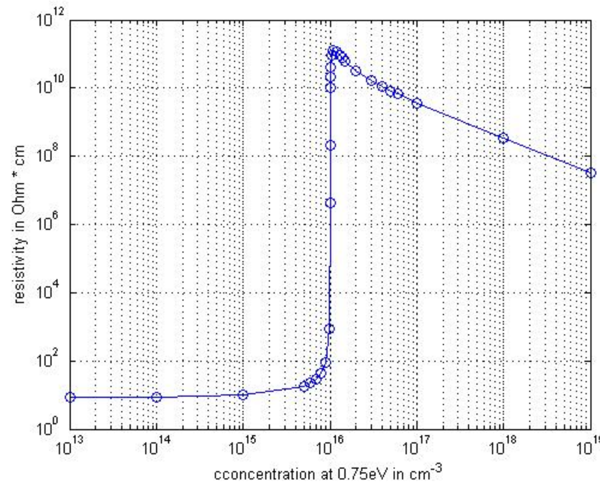

Fig. 2. Dependence of resistivity on deep level (0.75eV from conduction band) for the model of Ref [3].

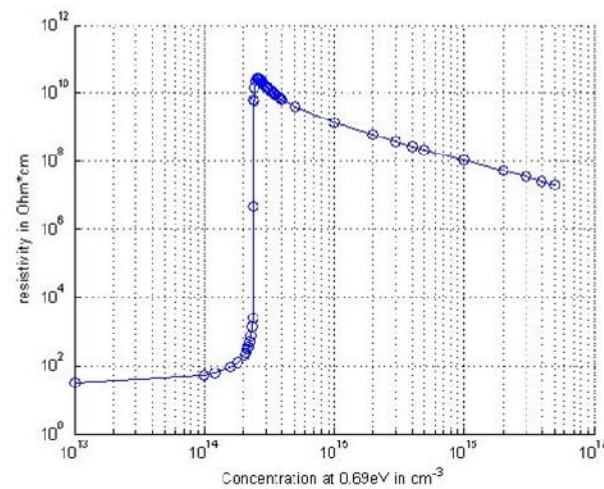

Fig. 3. Dependence of resistivity on deep level (0.69 eV from valence band) concentration for the model of Ref [4].

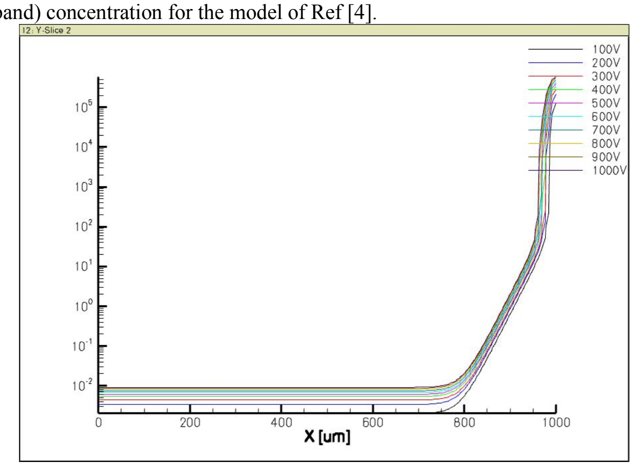

Fig. 4. Calculated electric field profile in V/cm inside a 2mm thick detector. Different positive bias voltages are applied on the electrode which forms a Schottky contact with the detector. The 0.69eV deep level concentration is $\cong 2 \cdot 10^{14}$

Obviously this is in contradiction with the fact that Schottky diodes made of Indium and of high resistivity p type CdTe crystals are used now routinely for spectroscopic applications. We would like to point out that the experimental investigations of the electric field profile inside high resistivity CdTe Schottky diodes give contradictory results, as can be seen in [5] and [6]. In order to be able to simulate the charge transport due to interactions with X-ray and gamma ray photons we reduced the deep level concentration to $10^{13} cm^{-3}$.

III. Transient Simulations of Charge Transport

For the transient simulations we used a detector with the geometry shown in Fig. 5. The pixel electrodes are of Ohmic type and the single electrode is of Schottky type. Using SDEVICE one has the possibility to define a certain region of the material where at some initial time electrons and holes are created. This can be used to simulate the conversion of a single X or gamma photon to charge due to the photoelectric effect.

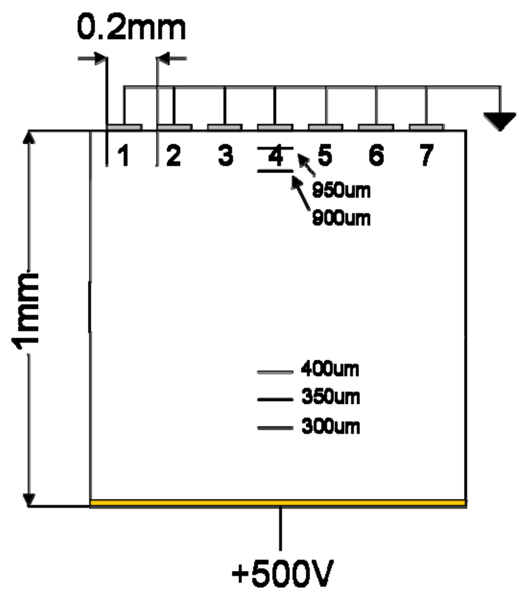

Fig.5. The pixel detector used in charge transport simulations. The single electrode has the Indium work function and forms a Schottky junction with the p-type low resistivity CdTe crystal. The bias voltage is set at 500V and the charge is delivered at distances from 300um to 950um from the single electrode.

The total current signal induced on each electrode from a photon conversion that delivered 12 fCb at a depth of 250um below the 4th electrode (750um from the single electrode) is shown in Fig. 6. In Fig. 7 we plot the ratio of the charge collected at the central electrode to the charge collected at the neighbor pixel for interactions occurring at different depths. It is clear that the ratio of the collected charges at different electrodes can be used as an indicator of the depth of interaction.

IV. Conclusions

From our work it is clear that for the modeling of the charge transport properties of CdTe the compensation models have to be modified in order to obtain high resistivity material with 1 to 4 orders of magnitude less concentration of the deep level.

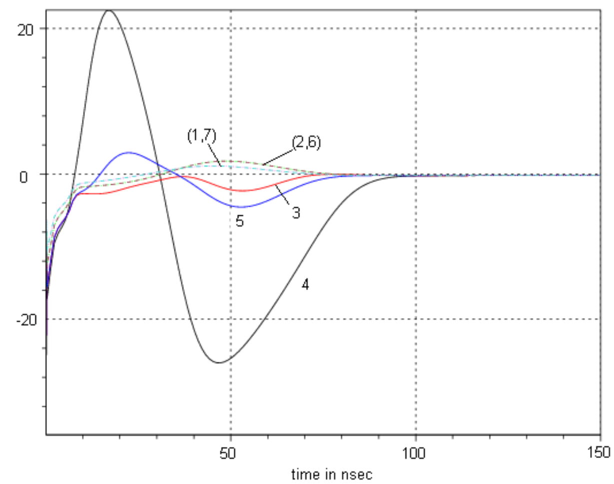

Fig. 6. Total current waveforms in nA at the pixel electrodes resulting from 12 fCb charge delivered at a distance of 750um from the cathode electrode.

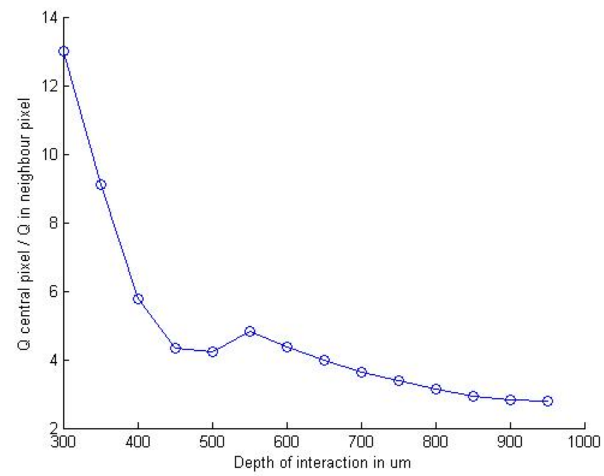

Fig. 7. Ratio of the charge collected at the electrode 4 to the charge collected at the electrode 3 as a function of the distance from the cathode of the photon conversion.

The relation between the charges collected at neighbor pixels can be used to extract the depth of interaction information.

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