Impact of TCAD Model Parameters on Optical and Electrical Characteristics of Radiation-Hard Photodiode in 0.35 μm CMOS Technology

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Abstract—In this paper, a variability Design of Experiment (DoE) is performed on a radiation-hard photodiode structure in order to understand how the physical parameters of the device impact its spectral responsivity and dark current. The varied physical parameters describe the carrier mobility, lifetime, energy bandgap and recombination models. The electrical and optical performance of the device are simulated using TCAD software, as a function of varied physical parameters. The simulations are calibrated to the device measurements. The analysis of the design showed that the carrier lifetime is the most influencing parameter that impacts both the spectral responsivity and the dark current. Mobility parameters and Auger recombination parameters impact the spectral responsivity, while the energy bandgap at 340 K impacts the dark current. Finally, the model parameters that fit the measured dark current are obtained by the thorough variation simulations.

Keywords—Image sensor, Ionizing radiation, Radiation hardness, TCAD software, Parameter variability, Screening, Design of Experiment, Spectral responsivity, Dark current

I. INTRODUCTION

Semiconductor detectors come in different varieties, like charge-coupled device (CCD) and CMOS image sensor (CIS), and generally consist of a sensing device and a readout circuit [1]. CIS are becoming more and more popular due to their wide application range, especially in terms of high-radiation environments. There are hybrid versions of a CIS, where the sensing device and the readout circuit are made on separated wafers and afterwards are bonded together. Due this processing, the hybrid CIS offers a large fill factor, and as the sensor and the readout circuit are independently optimized the other advantage is high radiation hardness. Their main disadvantage is the expensive and complex processing and production. On the other hand, the monolithic active pixel sensors (MAPS) are CMOS compatible which simplifies their production, as well as makes it cheaper. Their main disadvantage is the low operating voltage required for the CMOS readout circuit, and because of that the large depletion region is not achieved, thus reducing the charge collection efficiency and reducing the radiation hardness of the sensor. To overcome this issue, depleted MAPS (DMAPS) use the implementation of a high-resistivity starting material in

order to get a large depletion region and increase the charge collection efficiency and radiation hardness [2] [3]. Overall, CIS are used in radiation environments, especially for medical purposes and space applications. In medical applications, specifically in the Computed Tomography (CT) scanner, X-rays are used during the scan. The X-rays cause ionization damage, creating positive traps in the oxide and interface states near the silicon/silicon-oxide interface. These defects impact the recombination rate and trapping of the charge carriers, thus reducing the spectral responsivity, increasing the dark current and degrading the overall performance of the sensor [4] [5]. High radiation hardness can also be achieved by using a special high-lifetime starting material, where the charge collection is dominated by diffusion due to the large diffusion length. As the depletion region area is small, the capacitance is reduced, but the collection speed is then limited because it is dominated by diffusion and not drift effects.

The goal of this paper is to calibrate the TCAD model parameters in simulations of a photodiode structure with high-lifetime epitaxial layer intended for the use in X-ray detectors. The photodiode's spectral responsivity and dark current are simulated as a function of varied recombination, mobility and energy bandgap parameters and are compared to the measurements. The main impact on recombination rate have carrier lifetimes and their impact on photodiode characteristic are examined by TCAD simulations [6]. Moreover, carrier mobility impacts the diffusion length which is a crucial parameter if the charge collection is dominated by diffusion. As the photodiode is implemented in the CT scanner, the range of the operating temperature of the device is between 27 °C and 67 °C, so the energy bandgap parameters are also varied in the statistical design.

II. SIMULATED PHODIODE STRUCTURE AND PARAMETER VARIABILITY

The photoactive area of the photodiode is 565 μm x 795 μm , and consists of multiple n-well islands that act as the collection electrodes for the photo-generated charge.

Fig. 1. Cross-section of the simulated photodiode under the reverse voltage of 1.25V. The photodiode consists of a small n-well island that is surrounded by shallow p-type passivation layer. It is positioned in the high-lifetime p-type epitaxial layer, which was thermally grown on top of the low resistivity p-type substrate material.

A. Photodiode structure

The photodiode is fabricated in an industry standard 350 nm high-voltage (HV) CMOS technology and simulated using TCAD software. The resulting 2D cross-section is shown in Fig. 1. Model parameters used in fabrication sequence simulations are calibrated with the actual process. The I-V and spectral responsivity characteristics of the photodiode structure are then analyzed by device simulations.

Fig. 2 presents the comparison of the measured and initially simulated I-V curve of the photodiode using default TCAD parameters. The dark current was normalized to 1 island and is below 1 pA. Fig. 3 presents the comparison between measured and simulated spectral responsivity curves.

B. Parameter variability

In order to calibrate the simulations with the measured data, variation of different physical parameters has been performed. The simulations of these varied parameters give information on how each parameter impacts the spectral responsivity and the dark current.

Fig. 2. Comparison of the normalized measurement and simulated I-V curve using default TCAD parameters of the photodiode structure. The normalization was done by dividing the measurement values by the total number of n-well islands used in the photodiode. The measurement was performed at 340 K and the operating voltage was 1.25V in reverse bias.

Fig. 3. Comparison of the measured and simulated spectral responsivity curves of the photodiode structure.

The energy bandgap is calculated in simulations according to:

$$E_g(T) = E_{g0} + \delta E_{g0} + \frac{\alpha T^2}{\beta + T} \quad (1)$$

where T is temperature, E_{g0} is energy bandgap at 300 K and parameters $\alpha = 4.73 \cdot 10^{-4}$ eV/K and $\beta = 636$ K.

Doping dependent mobility of electrons is modeled by the Masetti model:

$$\mu_{dop} = \mu_{min1} + \frac{\mu_{const} - \mu_{min2}}{1 + \left(\frac{N_{A,0} + N_{D,0}}{C_r}\right)^\alpha} - \frac{\mu_1}{1 + \left(\frac{C_s}{N_{A,0} + N_{D,0}}\right)^\beta} \quad (2)$$

where μ_{min1} , μ_{min2} , μ_1 are reference mobilities, C_r , C_s are reference doping concentrations, α , β are the exponents μ_{const} is the low-doping reference mobility and $N_{A,0}$ and $N_{D,0}$ are acceptor and donor concentrations [7].

SRH parameters are modeled by the Scharfetter relation:

$$\tau_{dop}(N_{A,0} + N_{D,0}) = \frac{\tau_{max}}{1 + \left(\frac{N_{A,0} + N_{D,0}}{N_{ref}}\right)^\gamma} \quad (3)$$

where $N_{ref} = 10^{16} \text{ cm}^{-3}$ is the reference doping profile and the exponent, $\gamma = 1$. As the electron effective mass is lower than the hole effective mass, electron mobility is higher than the hole mobility. Because of that, the diffusion length for electrons is larger than for holes. Also, the lifetime of electrons is higher than lifetime of holes [8]. In TCAD it was modeled so that hole lifetime is one third of the electron lifetime.

Auger recombination is modeled in TCAD by:

$$R_{net}^A = (C_n n + C_p p)(np - n_{i,eff}^2) \quad (4)$$

where n , p are electron and hole concentrations respectively and the $n_{i,eff}$ is the effective intrinsic concentration. In the equation, parameters C_n and C_p are dependent on the Auger parameters and are calculated according to:

$$C_x(T) = \left(A_{A,x} + B_{A,n} \left(\frac{T}{T_0} \right) + C_{A,n} \left(\frac{T}{T_0} \right)^2 \right) \left[1 + H_x \exp \left(-\frac{x}{N_{0,x}} \right) \right] \quad (5)$$

where x represents electrons (n) or holes (p) depending on whether electrons or holes are used.

In Table I, parameters with their initial values are shown. The parameters are placed in four groups, where each group describes different physical settings: energy bandgap, doping dependent mobility, Shockley-Read-Hall (SRH) recombination, Auger recombination. In addition to those parameters, as the photodiode is used in the CT scanner, where the operating temperature goes up to 67 °C (340 K), simulations are also performed at 320 K (spectral responsivity) and 340 K (spectral responsivity and dark current).

III. DESIGN OF EXPERIMENTS AND RESULTS

In order to see the impact of the above mentioned parameters, the calibration methodology shown in Fig. 4 has been used. The block diagram of the calibration methodology consists of multiple steps. First, the parameters are varied in a wide range to see whether they impact the observed responses. Parameter screening is then performed, where these parameters are varied and sorted out according to the impact they have on photodiode

Table I. Simulation input parameters and their initial values. Parameters are shown in 4 groups that describe energy bandgap, doping-dependent mobility, SRH recombination and Auger recombination settings.

Variability table		
Group	Parameter	Value
Energy bandgap	E_{g0}	1.16964 eV
Doping dependent mobility of electrons	μ_{min1}	52.2 cm ² /Vs
	μ_{min2}	52.2 cm ² /Vs
	μ_I	43.4 cm ² /Vs
	C_r	$9.68 \cdot 10^{16}$ cm ⁻³
	C_s	$3.43 \cdot 10^{20}$ cm ⁻³
	α	0.68
	β	2
SRH recombination	τ_{maxE}	1 ms
	τ_{maxH}	one third of τ_{maxE}
Auger recombination	A_{AE}	$6.7 \cdot 10^{-32}$ cm ⁶ s ⁻¹
	A_{AH}	$7.2 \cdot 10^{-32}$ cm ⁶ s ⁻¹
	B_{AE}	$2.45 \cdot 10^{-31}$ cm ⁶ s ⁻¹
	B_{AH}	$4.5 \cdot 10^{-33}$ cm ⁶ s ⁻¹
	C_{AE}	$-2.2 \cdot 10^{-32}$ cm ⁶ s ⁻¹
	C_{AH}	$2.63 \cdot 10^{-32}$ cm ⁶ s ⁻¹
	H_{AE}	3.46667
	H_{AH}	8.25688
	N_{0E}	10^{18} cm ⁻³
	N_{0H}	10^{18} cm ⁻³

electrical and optical characteristics. The analysis of the Design of Experiment (DoE) shows the variability of the simulated responses as a function of the varied parameters such that the simulations could be calibrated with the measurements.

In the first set of simulations, a study of the impact of each parameter within their physically defined range of variations is performed. The study highlights the relative contribution of each parameter to the responses considered. As an example, the effect of varying the parameter α , ranging from 0.374 to 0.986, and implemented in the doping dependent mobility equation (2), is shown in Fig. 5. It can be seen that the SR curve decreases in values as the parameter increases, as it impacts the total doping concentration in the denominator of mobility equation. Basically, for larger α values, mobility is reduced, and therefore the diffusion constant of the carriers is also reduced. This means that the carriers recombine at shorter distance, and less charge is then collected by the collection electrode, which can be seen in reduced SR values. It can be noted that the variability of this parameter mostly influences lower and higher spectrum region. The absorption of the photons is determined by the absorption coefficient. For lower wavelengths, absorption of the photons is closer to the surface of the photodiode where the space charge region is placed. In that region, the doping levels are higher, either in n-well or in p-passivation region implying a smaller mobility and a higher impact of α for the same physical distance. For higher wavelengths, light is absorbed deeper in the structure, in the region with the out-diffusion from the substrate into the epitaxial layer. The absorption region is further away from the collection electrode, and because of that the diffusion length and hence the charge carriers are more likely to recombine before reaching the depletion region. Therefore, the mobility has a higher impact in the higher wavelength spectrum region (800-900 nm).

Fig. 4. Block diagram of the calibration methodology. Based on the DoE, Response Surface Model (RSM) is created which gives statistical parameter variability according to the quadratic relation of the input parameters.

Fig. 5. Impact of different α values from equation (2) on the spectral responsivity simulation at 340 K. Parameter α is ranging from 0.374 to 0.986.

After the first set of simulations, a screening design using the L24 Plackett and Burman model [9] has been generated and simulated. The screening percentages of all input parameters are selected such that the parameter values are in physical range of their initial values. According to the Table II, each value was screened with the tolerances compared to the initial values. This screening model was then imported in TCAD software and was simulated [10]. Analysis of the screening model provided a Pareto graph shown in Fig. 6. It indicates the importance of the impact of each parameter on the spectral responsivity (at 320 K and 340 K, and at 500 nm and 900 nm) and the dark current (at 340 K and 1.25 V). It can be observed that for spectral responsivity, the largest effect comes from the lifetime, mobility and auger parameter variability, and for the dark current, the largest impact has the energy bandgap variation as well as the lifetime variations.

Table II. Screening percentage of all input parameters according to the parameter group.

Screening percentage			
Energy bandgap	Doping dependent mobility of electrons	SRH recombination	Auger recombination
+/- 1.50%	+/- 20%	+/- 5000%	+/- 20%

Fig. 6. Pareto graph for the screening analysis.

After the analysis, the parameters with the highest impact are selected. For the spectral responsivity, τ_{maxE} , α , μ_{min1} , A_{AH} , C_r and N_{OE} parameters were selected as the most important parameters and for the dark current, E_{g0} and τ_{maxE} were selected. The other parameters are neglected as they have a considerably smaller effect either on spectral responsivity or on dark current. According to a central composite full design (with face centered) a response surface model (RSM) was designed. It is designed by taking into account the screened values and also the initial value. The RSM gives information on how the observed responses behave according to a quadratic function of the most relevant parameters. The sensitivity analysis of each parameter is obtained by RSM techniques that deliver the variability of each response according to the variation of the input parameters within their range. After the sensitivity analysis, calibrated parameter values that achieve the best fitting of spectral responsivity have been extracted, and are shown in Table III. The variability of the spectral responsivity as a function of the variability of τ_{maxE} , at 340 K in comparison with the normalized measurement, is shown in Fig. 7. Lifetime has the highest impact in the higher wavelength spectrum region (800-900 nm), as it affects recombination rate and for lower lifetime, recombination increases, leading to the degradation in spectral responsivity. In general, the effect of other varied parameters is quite low, and additional calibration, where geometrical and physical parameters are adjusted, is needed [11]. The sensitivity analysis of RSM for the dark current is shown in Fig. 8. It can be noted that the calibrated curves match the measured curve quite accurately.

Table III. Calibrated parameter values for spectral responsivity simulation.

Parameter	Initial value	Calibrated value
μ_{min1}	52.2 cm ² /Vs	62.64 cm ² /Vs
C_r	9.68·10 ¹⁶ cm ⁻³	11.6·10 ¹⁶ cm ⁻³
α	0.68	0.544
τ_{maxE}	0.001 s	0.05 s
A_{AH}	7.2·10 ⁻³² cm ⁶ s ⁻¹	5.76·10 ⁻³² cm ⁶ s ⁻¹
N_{OE}	10 ¹⁸ cm ⁻³	0.8·10 ¹⁸ cm ⁻³

Fig. 7. Variation of spectral responsivity as a function of variability of the electron lifetime.

Fig. 8. Sensitivity analysis of dark current: comparison between measurement, initial simulation and final simulation with the calibrated parameters.

IV. CONCLUSION

A variability method is presented where parameters that describe energy bandgap, SRH recombination, carrier mobility and Auger recombination are varied in order to understand how each parameter impacts the spectral responsivity and the dark current of the examined photodiode. Analysis of the statistical methodology showed us that carrier lifetime and mobility have the highest impact on the spectral responsivity and that the measured dark current can be fitted only by adjusting the electron lifetime. The variability of spectral responsivity as a function of carrier lifetime variability showed the range of responsivity values around the calibrated point, which is determined by the calibrated lifetime value. As the other parameters have small effect on spectral responsivity, additional calibration where geometrical and physical parameters are adjusted, is needed to fully calibrate the spectral responsivity. Additionally, this study have shown which model parameters has the highest impact on I-V and optical responsivity characteristics of silicon photodiodes. It can give the guidelines to the designer to optimize the substrate material and those fabrication steps that can impact the most important parameters. Moreover, it also provides the information of which parameters must be calibrated most accurately during the simulations of such photodiodes.

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