Simulation of surface radiation defects leakage current SiPM using Synopsys TCAD

P P Parygin*, E V Popova and V M Grachev
National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Kashirskoe highway 31, Moscow, 1125409, Russia
E-mail: donkarloson@gmail.com

Abstract. Synopsys TCAD is a professional software for the development of the semiconductor technological process and device simulation. In order to study a radiation damage of the surface of silicon photomultipliers (SiPMs), the simulation of these devices using Synopsys TCAD has been made. Experimental samples were produced by KETEK GmbH and have been irradiated with the different doses of X-rays with an energy of $E \approx 12$ keV. The current-voltage characteristics below breakdown measured before and after irradiations have been simulated with TCAD. Obtained curves for experimental and simulation data are presented.

1. Introduction
SiPMs are very promising semiconductor single photon sensitive devices with a high gain [1]. As opposed to conventional vacuum tube photomultipliers (PMTs), SiPMs are not sensitive to the magnetic fields, need much lower bias voltage and they are compact. SiPM is an array of connected in parallel identical single pixels, each of which represents a p-n junction with a serial resistor. Each pixel operates in Geiger mode, when the bias voltage is higher than the breakdown voltage [2]. SiPM has a promising application in such science areas as a high-energy physics, nuclear medicine and astroparticle physics. However, the possibility of using SiPMs in some areas is limited by the radiation tolerance. SiPM radiation hardness is being studied for several years, for example in [3, 4, 5]. However, in such works no attempt was made to separate a bulk and surface damage. Recently, the investigation of the pure surface radiation damage has been started. Firstly, it has been done for the Hamamatsu MPPCs [6] and then for the SiPMs produced by KETEK GmbH [7]. Though the detailed analysis were done in these works, the simulation has not been performed.

Synopsys TCAD (Technology Computer-Aided Design) [8] is a powerful tool for the simulation of the semiconductor devices with an environment to analyze the simulation results. In this work, Synopsys TCAD was used to implement a simple design of SiPM to understand the surface radiation damage in SiPM in more detail. Using this model, it is possible to make an analysis of the radiation influence on the surface and bulk regions with respect to surface electric field distribution.

2. Experimental samples and setup
KETEK GbmH (Munich, Germany) [9] manufactured experimental SiPM samples and test structures. Test devices (PNCV) represent a single pixel with p$^+$-type entrance window (1x1 mm$^2$) surrounded by n-type highly doped periphery with different gap from 62 µm to 152 µm on all four sides. The full
structure size is 1.1x1.1 mm². In this work the PNCV p-on-n structure with multilayer dielectric on top between p⁺-type and n-type (thermal oxide, silicon nitride and deposited oxide) were used. Keithley 6517B Electrometer [10] was used for the current-voltage characteristic measurements. All measurements were performed under normal conditions. X-ray irradiations were carried out using PHYWE XRE 4.0 Expert Set [11] with anode made of tungsten. Two different doses were applied on the test samples: 200 Gy and 3 kGy, using X-rays with an energy of E≈12 keV. The maximum transmitted energy to silicon atoms for 12 keV photons is 0.011 eV, which is quite below the damage threshold for silicon of 21 eV [12]. Thus, no bulk damage is expected for 12 keV photons. The irradiation of the samples were performed without biasing and the samples were not annealed after the irradiation. The current-voltage characteristics of the irradiated samples were measured immediately after the irradiation.

3. Simulation model

The PNCV SiPM model is presented in figure 1. This structure has a length $L = 20 \mu m$ and 5.5 $\mu m$ depth. It consists of the next layers: dielectric layer, which is presented, for simplification, as the single silicon dioxide (0.5 $\mu m$ depth), boron highly doped p⁺ entrance window (0.45 $\mu m$ depth), phosphorous n-type layer (2.5 $\mu m$ depth) performed as a retrograde profile and phosphorous n⁺ highly doped substrate (from 3 to 5 $\mu m$ depth). For the device simulation, the bias and the ground contacts have been added. The bias contact extends beyond p⁺-layer on silicon dioxide for 7 $\mu m$.

![Figure 1. Model structure (sizes are given in text).](image)

The full PNCV structure was implemented as this small model due to the requirement of the fine grid on Si-SiO₂ interface and reduce the simulation time. So, in the depth direction the minimum grid spacing is 1nm that is caused by the thin (up to 10 nm) inversion or accumulation layer on the Si-SiO₂ interface. The minimal grid in the lateral direction is defined by the p⁺-n junction and equals to 10nm.

The simulation of the model was performed in Synopsys Sentaurus Device tool for the currents before breakdown. For the current-voltage simulation, the drift-diffusion mode was applied to the system of equations consisting of nonlinear Poisson equation and continuity equations for electrons and holes [13]. Thus, the impact ionization was not used in the simulations. The velocity saturation was taken into account, and for the electric field intensity higher than $10^4$ V/cm the saturation velocity is $10^7$ cm/s.

For the generation-recombination processes, the Schockley-Read-Hall (SRH) recombination was used. In simulations it appears as SRH recombination for the bulk and surface regions (equations (1)).

$$R_{\text{bulk}}^{\text{SRH}} = \frac{np - n_i^2}{\tau_p (n + n_i) + \tau_n (p + p_i)}$$

$$R_{\text{surf}}^{\text{SRH}} = \frac{np - n_i^2}{(n + n_i) / S_p + (p + p_i) / S_n}$$

(1)

where $n(p)$ – electron (hole) density, $n_i$ – intrinsic concentration, $n_i$ ($p_i$) – donor (acceptor) trap concentration (see equations (2)), $\tau_n$ ($\tau_p$) – electron (hole) lifetime, $S_n$ ($S_p$) – electron (hole) surface recombination velocity.

$$n_1 = n_0 e^{E_{\text{trap}} / kT}$$

$$p_1 = n_0 e^{-E_{\text{trap}} / kT}$$

(2)
where $E_{\text{trap}}$ – trap energy level, $k$ – Boltzmann constant, $T = 293$ K – temperature. $E_{\text{trap}}$ value is the deviation of the trap energy level from the middle of the bandgap and it is equal to 0 in our case.

For the bulk SRH recombination we set $\tau_n = \tau_p = 1 \times 10^{-2}$ s for the non-irradiated and irradiated sample simulations. For the surface SRH recombination Synopsys TCAD simulates surface recombination velocities $S$ taking into account their doping dependencies according to equation (3):

$$
S = S_0 \left[ 1 + S_{\text{ref}} \left( \frac{N_s}{N_{\text{ref}}} \right)^\gamma \right]
$$

(3)

where $S_0$ – surface recombination parameter, $S_{\text{ref}} = 1 \times 10^3$ – reference value of surface recombination velocity, $N_s$ – ionized dopant concentration, $N_{\text{ref}} = 1 \times 10^{16}$ cm$^{-3}$ – reference value of ionized dopant concentration, $\gamma = 1$ – degeneracy factor.

Also, we used a simplified model of the Si–SiO$_2$ interface charge. It represents a sum of an oxide charge and interface traps charge. The latter one depends on the type (donor or acceptor), energy level and Fermi energy level [14, 15]. The charge and surface recombination velocity values are different for the non-irradiated and irradiated sample simulations.

4. Results

The test simulations for the “short” ($L = 20$ µm) and “long” ($L = 160$ µm) structures were performed in order to confirm that there is no significant influence on the result currents for different charges and $S_0$ (figure 2).

![Figure 2: Comparison of the short and long model currents.](image)

In order to separate the bulk and surface currents, we performed two simulations. In the first case, the surface generation-recombination processes were deactivated and the only bulk current has been obtained. In the second one, we activate only the surface physical models and deactivate the bulk ones, and as a result, we have the pure surface current. Our model is two-dimensional and, by default, Sentaurus Device assumes a “thickness” (width along z-axis) of 1 µm.

Bulk currents was scaled using coefficient depends on the entrance window area ratio between the model and real PNCV structure. For the surface currents, the periphery perimeter ratio coefficient was used. The full current is equal to the sum of the scaled currents. However, the bulk current is much
lower than surface one (figure 3a). It is consistent with data reported in [16]. This model of the current calculation was applied to both non-irradiated and irradiated simulations too.

Figure 3. a) bulk and surface currents comparison according to non-irradiated sample; b) influence of the interface charge on I–V curve with constant surface recombination velocity (200 Gy example); c) influence of surface recombination velocity on I–V curve with constant charge (200 Gy example). Experimental errors are within the data points.

The simulation of the irradiated samples were performed with the same bulk lifetime as for non-irradiated samples (since there is no bulk damage), but within creasing the charge in the Si–SiO2 interface and the surface recombination velocity. Using the different interface charges we are able to adjust the shape of the I–V curve (figure 3b). With surface recombination velocity, it is possible to move up and down the curve so we can reach the required current values as it is shown in figure 3c. For the irradiated samples, the positive charge does not fit and the negative charge [17] was used.

The results of the comparison of the current-voltage characteristics for the simulated and produced sample can be seen in figure 4. The curves are presented for the non-irradiated samples and the samples irradiated with 200 Gy and 3 kGy doses. As one can see, the shape of the simulated and experimental I–V characteristics for the non-irradiated samples is similar, but there is a slope of the simulation curve after some point. It could be caused by the simplicity of the simulation model. As concerns irradiated samples, the shapes and the values of the simulated current-voltage characteristics are in the good agreement with experimental data. The obtained values of the parameters are presented in table 1.

Table 1. The results parameters for the non-irradiated and irradiated samples.

| Interface charge, C   | S₀, cm/s |
|----------------------|---------|
| 0 Gy                 | +1⋅10¹¹| 0.02   |
| 200 Gy               | -8.3⋅10¹¹| 8.0    |
| 3 kGy                | -2⋅10¹² | 230.0  |

Figure 4. Comparison of experimental and simulation data, a) for non-irradiated samples; b) for 200 Gy dose; c) for 3 kGy dose.
5. Conclusion
In this work, an attempt to model the Silicon photomultipliers with Synopsys TCAD was presented. The simulation results were compared with the PNCV samples manufactured by KETEK GmbH. Using developed model, it is possible to obtain the amount of the charge located on Si-SiO$_2$ interface and the value of the surface recombination velocity of SiPM. Further work is being started and it concerns the simulation of the complete SiPM.

Acknowledgement
The work has been partially supported by Megagrant 2013 program of Russia, agreement № 14.A12.31.0006 from 24.06.2013 and partially supported by Institute for Experimental Physics, Hamburg University and partially supported by MEPhI Academic Excellence Project (contract № 02.a03.21.0005, 27.08.2013).

Especially, we thank prof. Erika Garutti and Dr. JoernSchwandt from Hamburg University for helpful advices and discussions.

References
[1] Buzhan P et al. 2003 Silicon photomultiplier and its possible applications Nucl. Instrum. Meth. A 504 48–52
[2] Dolgoshein B et al. 2001 An Advanced Study of Silicon Photomultiplier ICFA Instrumentation Bulletin 23 28–41
[3] Danilov M 2007 Nucl. Instrum. Meth. A 581 451
[4] Musienko Y et al. 2007 Nucl. Instrum. Meth. A 581 433
[5] Musienko Y et al. 2015 Nucl. Instrum. Meth. A 787 319–22
[6] Xu C et al. 2014 Influence of X-ray irradiation on the properties of the Hamamatsu silicon photomultiplier S10362-11-050C Nucl. Instrum. Meth. A 762 149–61
[7] Garutti E et al. 2014 Silicon photomultiplier characterization and radiation damage investigation for high energy particle physics applications JINST 9(3) C03021
[8] Synopsys TCAD (http://www.synopsys.com/tools/tcad/)
[9] KETEK GmbH (http://www.ketek.net/)
[10] Keithley 6517B (http://www.keithley.com/products/dcac/sensitive/highresistance/?mn=6517B/)
[11] PHYWE XRE 4.0 (http://www.phywe.com/en/09110-88/)
[12] Akkerman A et al. 2001 Updated NIEL calculations for estimating the damage induced by particles and gamma-rays in Si and GaAs Radiation Physics and Chemistry 62 301
[13] Synopsys Sentaurus Device manual 2012
[14] Schwandt J et al. 2012 Optimization of the radiation hardness of silicon pixel sensors for high x-ray doses using TCAD simulations JINST 7 C01006 (arXiv:1111.4901)
[15] Zhang J et al. 2012 Investigation of X-ray induced radiation damage at the Si-SiO2 interface of silicon sensors for the European XFEL JINST 7 C12012 (arXiv:abs/1210.0427)
[16] Engelmann E et al. 2015 Extraction of activation energies from temperature dependence of dark currents of SiPM (in this proceedings)
[17] Warren W L et al.1993 Journal of Applied Physics 74 4034