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# TCAD modeling of bulk radiation damage effects in silicon devices with the Perugia radiation damage model

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## ABSTRACT

The "Perugia Surface and Bulk" radiation damage model is a Synopsys Sentaurus Technology CAD (TCAD) numerical model which accounts for surface and bulk damage effects induced by radiation on silicon particle detectors. In this work, the significance of the input parameters of the model, such as electron/hole cross sections and acceptor/donor introduction rates is investigated, with respect to the changes in leakage current, full depletion voltage, charge collection efficiency and the current-related damage factor $\alpha$ (an irradiated device's figure of merit) of a PIN diode. Different types (IV, $1/C^2$-V) of comparisons are made between simulation outputs and experimental data taken from irradiated PIN diodes. Finally, the possibility of the analytical model's validation with the examination of the Low-Gain Avalanche Detector (LGAD) case, and its general application for future silicon sensors is discussed.

## 1. Introduction

During the High-Luminosity (HL) era, the innermost layers of the LHC tracker detectors, such as ATLAS and CMS, will have to withstand fluences higher than 2E16 $n_{eq}/cm^2$ and total ionizing doses (TID) of the order of 10 MGy (1 Grad) over 10 years of data taking [1]. For this reason, effective and radiation-resistant detectors fulfilling the technical specifications required for this extreme operating scenario need to be designed. Low-gain avalanche diodes (LGADs) are some of the most promising devices to cope with the high spatial density of the HL era and to achieve the timing resolution required in order to distinguish tracks belonging to different vertexes [2]. An LGAD can be viewed as a PIN diode with an additional p-doped implant, the so-called gain layer (GL), surrounded by a junction termination extension (JTE) structure. Under full depletion, the p-doped implant generates a high-electric-field region near the detector surface. Electrons drifting towards the cathode (front side) are accelerated by the high electric field and subsequently an avalanche takes place due to the impact ionization. Taking advantage of the controlled charge multiplication in silicon, the LGAD design yields low gain values and therefore low noise levels. Thanks to this, it is possible to improve the SNR limiting its drastic reduction with fluence. Consequently, a robust and reliable simulation framework for the reproduction of the experimental behavior of non-irradiated and irradiated LGADs and other sensors is required. It should be capable of reproducing the operation of silicon devices under extreme fluences (>1E17 $n_{eq}/cm^2$) in order to be used for the design of LGADs with thin active substrates, that could mitigate the increase of dark current and the trapping of charge carriers which decrease the charge collection efficiency [3]. In this work, we advance the fully implemented within the Synopsys Sentaurus TCAD suite of tools [4] "New University of Perugia TCAD model" (2021) [5], which aims to predict the LGADs' performance up to the extreme fluences expected in the future collider experiments and the corresponding radiation damage effects. Just like its predecessors, the latest versions of the numerical Perugia model describe both surface [6] and bulk damage effects in silicon devices [7] and implements the acceptor removal mechanism in the multiplication layer, which at the moment limits the use of LGADs above fluences of the order of 1E15 $n_{eq}/cm^2$ due to the deactivation of the acceptor dopant in the gain layer. The ultimate versions of the model, i.e. the ones presented in this study, are collectively called $PerugiaModDoping$ (2022), where an analytical modeling of the bulk doping has been implemented in the "New University of Perugia TCAD

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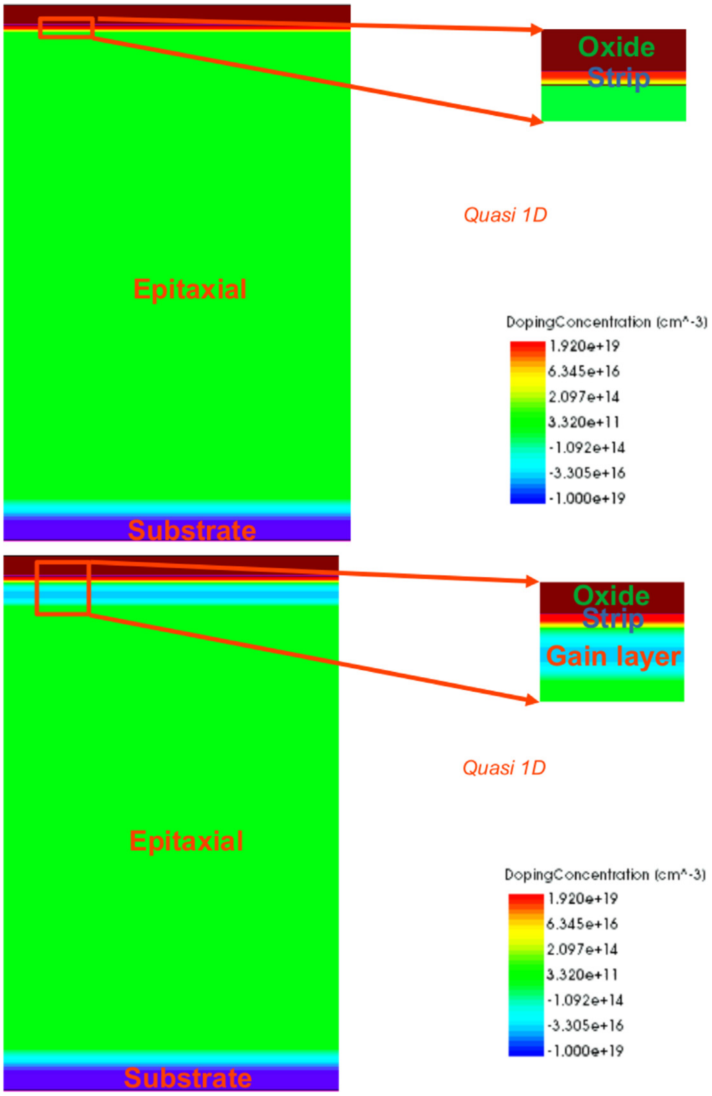


**Fig. 1.** The simulated structures of a PIN diode (top) and of an LGAD (bottom) for three different FBK geometries (a), (b) and (c). (1) Silicon: Width = 20 μm; thicknesses: (a) 25; (b) 35; (c) 55 μm: Epitaxial layer: (a) 24.5; (b) 34.5; (c) 50 μm; substrate: (a) 0.5; (b) 0.5; (c) 5 μm. (2) Silicon oxide: Width: 18 μm; thickness: 1 μm.

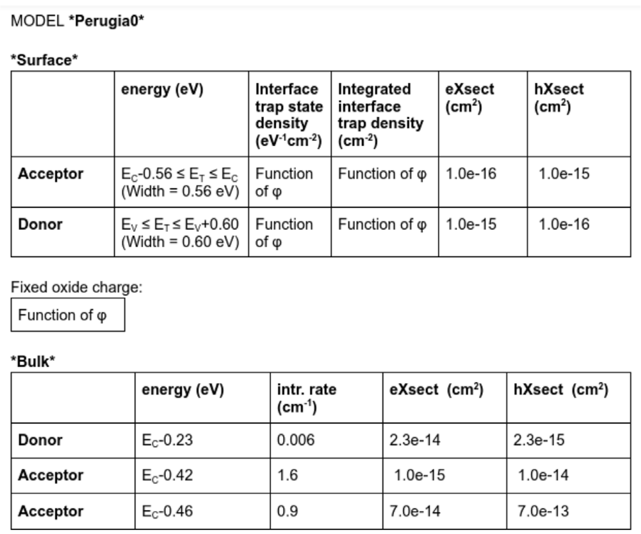
model" (in addition to the analytical modeling of the doping of the gain layer) in order to describe the acceptor creation mechanism at high ionization doses where saturation effects are observed. The new series of models have been fine-tuned on PIN data and subsequently validated on LGADs.

## 2. Devices and simulation model

The simulated structures in this study are based on sensors produced at Fondazione Bruno Kessler (FBK) in Trento, Italy. The electrical measurements were performed by the Turin and Perugia groups. The PIN diodes are diodes with a wide, undoped intrinsic silicon region between two heavily-doped ones, one of p-type and the other of n-type. The LGADs are similar to PIN diodes but with a p-doped implant serving as a Gain Layer (GL). Three distinct geometries corresponding to different silicon thicknesses were investigated for both the PIN diodes (Fig. 1, top) and the LGADs (Fig. 1, bottom), (a), (b) and (c), with the following parts in each of them: (1) Silicon: Width: 20 μm; Nominal thickness: (a) 25; (b) 35; (c) 55 μm: Epitaxial layer thickness: (a) 24.5; (b) 34.5; (c) 50 μm; Substrate thickness: (a) 0.5; (b) 0.5; (c) 5 μm. (2) Silicon oxide: Width: 18 μm; Thickness: 1 μm.

A starting point for the work presented here is the "Perugia Surface + Bulk" (2019) model [8] (our Perugia0 model for the current study), fully implemented within the Synopsys Sentaurus Technology CAD (TCAD) tool (Fig. 2). The driving force behind our studies is the need to describe the surface and bulk damage effects induced by radiation in silicon sensors relying on a limited number of parameters relevant for physics. The integrated interface trap density and the oxide charge density have been determined before and after X-ray irradiation with doses ranging from 0.05 to 100 Mrad ($SiO_2$) and relying on samples from different foundries and technologies (since the initial "Perugia 2019 Surface" model has been tested with the FBK, HPK and IFX devices). The next objective is to optimize the reproduction of the bulk damage effects.

During the fine-tuning of the new model, the capacitance–voltage (CV) simulations were in the general case performed at 300 K and for a 1 kHz frequency, while the current–voltage (IV) simulations were in the general case performed at 253 K and scaled using Chilingarov's formula $I(T) \propto T^2 \exp(-1.21\ \mathrm{eV}/2k_B T)$, where $I$ is the electric current, $T$ is the absolute temperature and $k_B$ is the Boltzmann constant [9]. The physical models used are Shockley–Read–Hall (SRH), Band-To-Band Tunneling (since when increasing the doping concentration, the peak current increases because of more carriers available for tunneling), Auger for the generation/recombination rates, e/h mobility and the Massey avalanche model [10] for the IV simulations, as well as the series of New University of Perugia models (for surface and bulk damage modeling) including a trap generation mechanism [11].



MODEL ***Perugia0***

***Surface***

| | **energy (eV)** | **Interface trap state density ($eV^{-1}cm^{-2}$)** | **Integrated interface trap density ($cm^{-2}$)** | **eXsect ($cm^2$)** | **hXsect ($cm^2$)** |
|---|---|---|---|---|---|
| **Acceptor** | $E_C$-0.56 ≤ $E_T$ ≤ $E_C$ (Width = 0.56 eV) | Function of φ | Function of φ | 1.0e-16 | 1.0e-15 |
| **Donor** | $E_V$ ≤ $E_T$ ≤ $E_V$+0.60 (Width = 0.60 eV) | Function of φ | Function of φ | 1.0e-15 | 1.0e-16 |

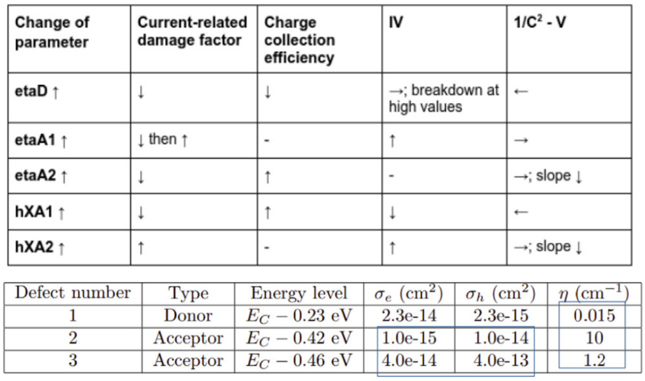
Fixed oxide charge:

Function of φ

***Bulk***

| | **energy (eV)** | **intr. rate ($cm^{-1}$)** | **eXsect ($cm^2$)** | **hXsect ($cm^2$)** |
|---|---|---|---|---|
| **Donor** | $E_C$-0.23 | 0.006 | 2.3e-14 | 2.3e-15 |
| **Acceptor** | $E_C$-0.42 | 1.6 | 1.0e-15 | 1.0e-14 |
| **Acceptor** | $E_C$-0.46 | 0.9 | 7.0e-14 | 7.0e-13 |

**Fig. 2.** The Perugia0 model developed in 2019 which combines surface and bulk radiation damage effects.



| **Change of parameter** | **Current-related damage factor** | **Charge collection efficiency** | **IV** | **1/C² - V** |
|---|---|---|---|---|
| **etaD ↑** | ↓ | ↓ | →; breakdown at high values | ← |
| **etaA1 ↑** | ↓ then ↑ | - | ↑ | → |
| **etaA2 ↑** | ↓ | ↑ | - | →; slope ↓ |
| **hXA1 ↑** | ↓ | ↑ | ↓ | ← |
| **hXA2 ↑** | ↑ | - | ↑ | →; slope ↓ |

| Defect number | Type | Energy level | $\sigma_e$ ($cm^2$) | $\sigma_h$ ($cm^2$) | $\eta$ ($cm^{-1}$) |
|---|---|---|---|---|---|
| 1 | Donor | $E_C - 0.23$ eV | 2.3e-14 | 2.3e-15 | 0.015 |
| 2 | Acceptor | $E_C - 0.42$ eV | 1.0e-15 | 1.0e-14 | 10 |
| 3 | Acceptor | $E_C - 0.46$ eV | 4.0e-14 | 4.0e-13 | 1.2 |

**Fig. 3.** A sensitivity analysis of various input parameters of the model (*etaD*: introduction rate for the donor level; *etaA*1: introduction rate for the first acceptor level; *etaA*2: introduction rate for the second acceptor level; *hXA*1: the capture cross section for the holes at the first acceptor level; *hXA*2: the capture cross section for the holes at the second acceptor level) and the impact of their change on the simulation outputs (top) and a best case scenario (called "best case 18") determined as the optimal one in terms of proximity to experimental data, where the changes compared to the Perugia0 model are inside the blue rectangles (bottom).

In all the new versions of the Perugia model there are always two acceptor levels and one donor level for the description of the bulk damage. Their energies $E$ are calculated from the conduction band $E_C$. The important input parameters are the introduction rate $eta$ ($\eta$), the mid-energy level of uniformly distributed band of traps $Emid$ and the capture cross sections for holes/electrons $hx/ex$ ($\sigma_h/\sigma_e$) for which the relations $exA = hxA/10$, $hxD = exD/10$, with $A$ standing for acceptor levels and $D$ standing for donor levels, are always imposed for convenience. A total of 18 new cases of the model were examined, where a different subset of the input parameters was varied in each of them. Through this sensitivity analysis, the trends of important simulation outputs and the effects caused by the modification of input parameters are summarized in Fig. 3, top. A best case (case 18) was determined as the one for which the sum of squares of relative differences between simulated and experimental values of all the important magnitudes is minimized. The best case 18 can be seen in Fig. 3, bottom. The acceptor-removal mechanism in the multiplication layer was implemented using the analytical law for the concentration $N_{GL}(\phi) = N_A(0)\exp(-c\phi)$, where $\phi$ is the fluence. According to it, the peak dose of the gain-layer profile, $N_{GL}$, is recomputed as a function of the fluence, the initial acceptor density $N_A(0)$ and a constant factor $c$, which is calculated from the so-called "Torino acceptor removal" parameterization [12]. It has been determined experimentally that the acceptor creation can be described by the following analytical bulk parameterization, now called "Torino acceptor creation" parameterization:

$$N_{A,bulk} = \begin{cases} N_{A,bulk}(0) + g_c\phi & 0 < \phi \leq 3\text{E}15\text{n}_{\text{eq}}/\text{cm}^2 \\ 4.17\text{E}13 \cdot \ln(\phi) - 1.41\text{E}15 & \phi > 3\text{E}15\text{n}_{\text{eq}}/\text{cm}^2 \end{cases} \quad (1)$$

where $g_c = 0.0237$ cm$^{-1}$ [13].

All results presented below are for a modified version of "Perugia 2019" where the doping concentration is a piecewise function. The model was named *PerugiaModDoping*. Initially, it was fine-tuned with data from PIN diodes and subsequently it was validated for LGADs. All magnitudes are presented in absolute values.

## 3. Results

Below we present the simulation outputs for the best case scenario of *PerugiaModDoping* which were obtained during the fine-tuning of the input parameters, along with the related comparisons with data from irradiated devices for which a fluence of 2E14 $n_{eq}/cm^2$ corresponds to approximately 10 Mrad (since for the CMS Outer Tracker the maximum fluence is 1E15 $n_{eq}/cm^2$ and the corresponding TID is 56 Mrad [14]). The simulated and experimental current–voltage (IV) curves of a 55 μm thick diode for different fluences are presented in Fig. 4. The current-related damage factor $\alpha$ is calculated from the slope of the respective ΔI/V vs fluence curve (where V is the volume). $\alpha = 7.872\text{E}{-17}$ A/cm for the *PerugiaModDoping* best case while $\alpha = 6.031\text{E}{-17}$ A/cm for the initial *Perugia*0 model. In Fig. 5, the simulated and measured 1/C$^2$ - V curves at three different temperatures

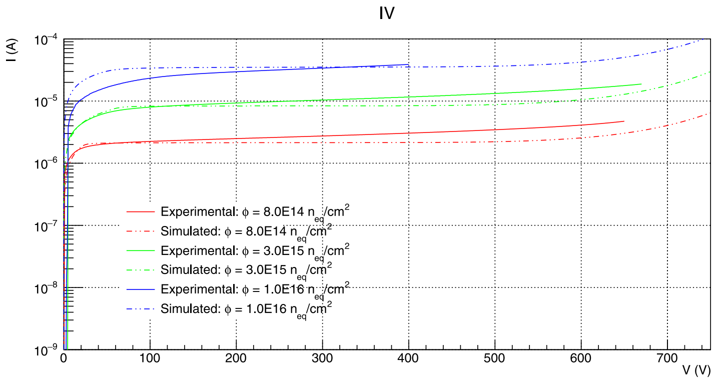


**Fig. 4.** Simulated with *PerugiaModDoping* current–voltage (IV) curves for a 55 μm thick PIN diode at various fluences and comparison with experimental measurements.

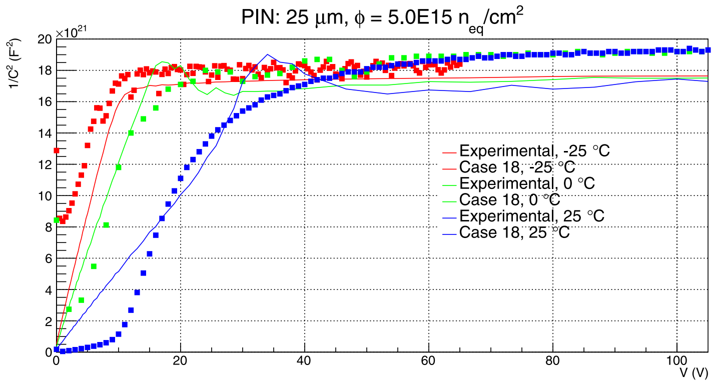


**Fig. 5.** Simulated with *PerugiaModDoping* and experimentally measured $1/C^2$ - V for a 25 μm thick PIN diode at different temperatures. All data for 5.0E15 $n_{eq}/cm^2$.

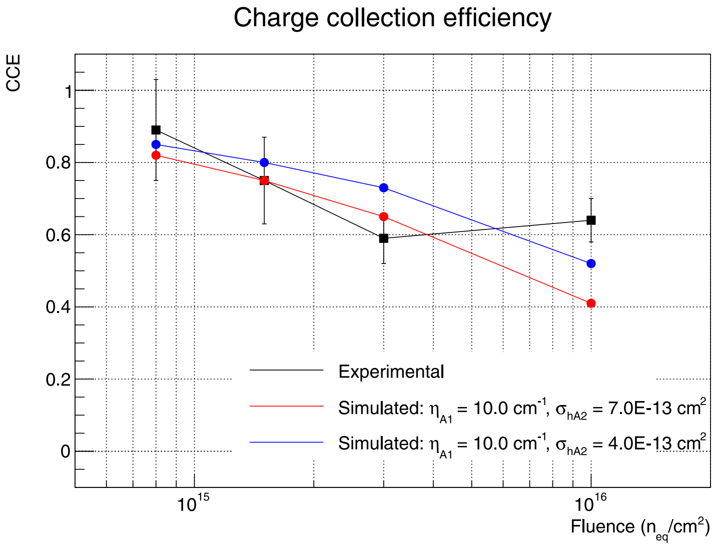


**Fig. 6.** Experimentally measured (black), simulated with a trial version of the model (case 6, red) and simulated with *PerugiaModDoping*'s best case (blue) charge collection efficiency (CCE) for a 55 μm thick PIN diode. Each measurement is taken at a bias voltage between 300 V and 500 V (absolute values) and the respective output value of the simulation is each time obtained at the same bias voltage as the experimental one. CCE = 1 for fluence = 0 $n_{eq}/cm^2$. Room temperature.

for a 25 μm thick PIN diode can be seen. The simulated (using the *PerugiaModDoping* and an intermediate version of the model) and experimental charge collection efficiency as a function of the fluence is displayed in Fig. 6 for a 55 μm thick PIN diode. After the best case was determined, the model was tested with LGADs of different geometries and for numerous temperatures, in terms of IV and $1/C^2$ - V curves, CCE and $\alpha$. The agreement is considered very satisfactory. Indicative comparisons between experimental data and *PerugiaModDoping*'s output are the $1/C^2$ - V curves for a 35 μm thick LGAD at various temperatures shown in Fig. 7 (where the variation of the full-depletion voltage with temperature is expected [15]) and the IV curves for a 55 μm thick LGAD at various fluences and room temperature shown in Fig. 8. Two peaks are observed at the electric field vs $Y$-coordinate (thickness dimension coordinate) curves, corresponding to the $Y$ at the gain layer and the substrate. (We do not demonstrate it here due to lack of space.)

## 4. Conclusions

In this study, the behavior of PIN diodes produced at FBK has been reproduced in Sentaurus TCAD simulations with a new series of Perugia models. Given that electrical measurements performed in Turin demonstrate a change in the acceptor doping concentration value with fluence, this novel parameterization has been incorporated into the simulation model. The impact of varying the input parameters of the model has been investigated and summarized. An optimal combination of input parameters (a best case), which gives a very good agreement between simulated and experimental results in terms of IV and $1/C^2$ - V curves, CCE calculation and $\alpha$ calculation, has been determined. The newly developed versions of the model (named *PerugiaModDoping*) have been tested for different PIN diode thicknesses and temperatures, as well as for fluences up to 1E16 $n_{eq}/cm^2$, with the addition of the "Torino acceptor creation" parameterization; and have subsequently been validated for low-gain avalanche diodes. As future steps, we intend to further fine-tune *PerugiaModDoping* in order to match the experimental data at even higher fluences [16], after performing the related electrical measurements on the irradiated PIN diodes and LGADs. The final model will be used during the design phase of future LGAD-based sensors (such as AC and DC-coupled resistive silicon detectors) and 3D detectors. Additionally, it can be a powerful tool for the simulation of sensors used in the upgraded LHC experiments.

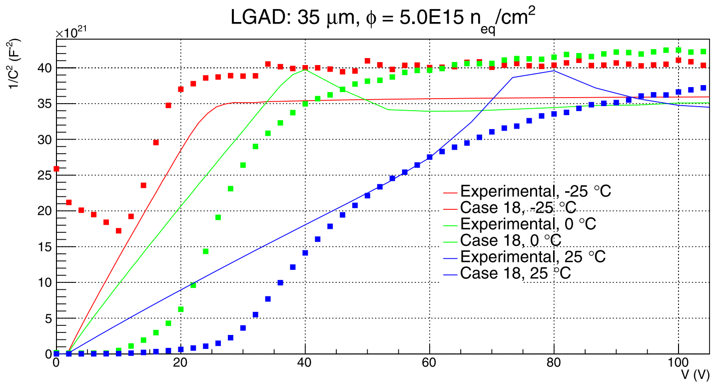


**Fig. 7.** Simulated with *PerugiaModDoping* and experimentally measured 1/C$^2$ - V curves for a 35 µm thick LGAD at different temperatures. All data for 5.0E15 n$_{eq}$/cm$^2$.

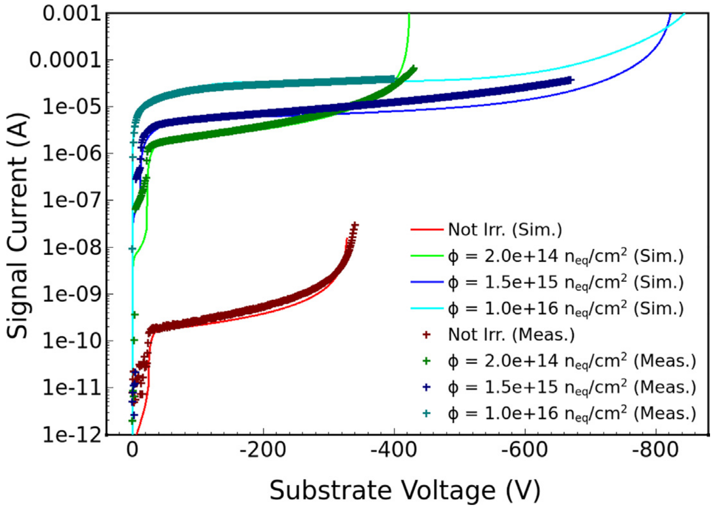


**Fig. 8.** Simulated with *PerugiaModDoping* and experimentally measured IV curves for a 55 µm thick LGAD at 300 K and different fluences.

## Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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