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TCAD simulations for radiation-tolerant silicon sensors

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Future High Energy Physics experiments require sensors to operate at extreme fluences exceeding 1×10^{17} 1 MeV n_{eq}/cm^2. Therefore, technologies used for the HL-LHC scenario will be no longer applicable and novel sensors and readout electronics must be devised. Within this framework, state-of-the-art Technology CAD tools can be proficiently used to account for the radiation-induced damage effects in semiconductor sensors, fostering design optimization and enabling predictive insight into the electrical behavior of novel solid-state detectors. Various numerical models addressing radiation damage effects have been developed and applied to the study of irradiated devices and will be illustrated in this work. Their applicability needs to be extended to extreme fluences accounting for the modeling of dopant removal, impact ionization, carriers' mobility and lifetime, and trap dynamics.

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1. Introduction

The next-generation colliders present formidable challenges in terms of energy and luminosity demands. Addressing radiation challenges requires radiation tolerant silicon sensors, capable of operating at extreme fluences exceeding 1×10^{17}1MeV n$_{eq}$/cm^2. Technologies used for the HL-LHC scenario will be therefore no longer applicable and radiation hardness becomes a paramount criterion for detectors and electronics, underscoring the need for a thorough investigation into radiation-induced damage effects with heightened awareness.

Within this framework, state-of-the-art Technology CAD (TCAD) tools have been proficiently used to account for the radiation-induced damage effects in semiconductor sensors. Several numerical models have been developed over the years to study and predict the behavior of specific sensor types irradiated with particular particle types up to the relevant fluences for the HL-LHC upgrade. These existing models must be extended to the extreme fluences to foster the design optimization and to enable predictive insight into the electrical behavior of novel solid-state detectors. Factors such as dopant removal, damage saturation, impact ionization, carriers' mobility and lifetime, and trap dynamics need to be carefully considered. The ultimate goal is to simultaneously reproduce and predict the macroscopic electrical behavior of silicon detectors in terms of Current-Voltage (I-V), Capacitance-Voltage (C-V), and Charge Collection Efficiency (CCE) at the fluences of interest in future collider experiments.

2. Radiation damage

The remarkable performance of silicon sensors in radiation environments has encouraged their extensive use in High-Energy Physics (HEP) applications, and forthcoming experiments foresee these sensors to operate at extreme levels of radiation. The detectors' macroscopic properties alter upon radiation exposure, significantly affecting their performance and emerging as the decisive factor dictating operational limits. Radiation damage in silicon detectors results in several effects, such as an increase in leakage current, bulk resistivity, space charge concentration, and trapping of free carriers. The increase in space charge concentration can substantially increase the sensor's full depletion voltage (V$_{FD}$), leading to potential breakdown when operated at high biases or loss of charge collection efficiency when operated at biases lower than full depletion. Beyond a fluence of 1×10^{16} n$_{eq}$/cm^2, a key limitation in silicon detector operation is the severe trapping of free carriers by radiation-induced defect levels. The semiconductor property changes at extreme fluences are very poorly known but represent a critical consideration for detector design and optimization. It is not possible to straightforwardly extrapolate the damage parameters to higher fluences, given the non-linear nature of the defect formation process with fluence [1, 2]. Additionally, the saturation of the radiation damage effects above 5×10^{15} n$_{eq}$/cm^2 needs to be taken into consideration.

Further efforts are crucial for characterizing radiation effects at extreme fluences to understand the limits of current models. Studying defects in irradiated sensors enables precise assessments of defect concentrations and trapping parameters using specialized spectroscopic techniques based on capacitance or current measurements (e.g., DLTS, TSC, TSCap) [3]. These methods provide essential insights into the features of radiation-induced defects, serving as key input parameters for numerical simulations of the sensor performance under diverse conditions. The new radiation level requirements demand suitable techniques for detecting defects above 1×10^{16}1MeV $\mathrm{n}_{eq}/\mathrm{cm}^2$. The knowledge gained, both existing and newly generated, will be utilized to develop advanced methods, methodologies, and numerical modeling schemes for the description of the radiation damage effects, aiming at optimizing the design of new generations of radiation hard detectors.

In the pursuit of enhancing the radiation hardness of silicon sensors for future experiments, there is a growing interest in investigating sensors characterized by novel designs and distinctive features. Intrinsic charge multiplication emerges as a viable strategy for mitigating the adverse effects of radiation damage, making LGAD-based devices optimal candidates for this purpose. In this direction, new challenges need to be addressed towards extending the charge carrier multiplication up to 1×10^{17}1MeV $\mathrm{n}_{eq}/\mathrm{cm}^2$.

3. TCAD Radiation damage modeling schemes

Radiation damage effects significantly affect the electrical performance of solid-state detectors both in terms of static (I-V, C-V) and active behaviors (CCE) depending on the irradiation level. A thorough comprehension of the macroscopic effects related to damage is essential for formulating a physics-driven numerical modeling scheme with predictive capabilities for the electrical behavior of irradiated silicon sensors.

Advanced TCAD simulation tools, operating at the device/circuit level, provide a range of approaches for analyzing semiconductor devices. These tools strike a balance between physical accuracy, comprehensiveness, application versatility, and computational demand. The TCAD simulation tools mainly solve the Poisson equation coupled with the current continuity equations for electrons and holes, typically considering the drift-diffusion current model. There is also the possibility to perform mixed-mode simulations including an external circuit connected to the device using the incorporated SPICE package, to predict e.g., read-out related waveforms. The simulation approach grants insight into the sensors operation, and both macroscopic and microscopic quantities, which are not accessible in experiments, can be evaluated. The available portfolio of approaches underscores the challenge of developing a reliable model capable of comprehensive prediction analyses. This is especially relevant when dealing with complex phenomena, such as the effects of radiation damage.

The development of a TCAD radiation damage model consists of specifying a series of defect states characterized by their type (i.e., donor or acceptor), concentration, energy level within the semiconductor bandgap, distribution (i.e., single level, uniform/gaussian band of defects), and capture cross-sections for electrons and holes. The goal is to reproduce the effects of the radiation damage and not the causes. Therefore the widely acknowledged approach within the scientific community is to select only a limited number of effective defect states. The currently available radiation damage models are described in the next sections. They differ in terms of defect description and they are often tailored to specific datasets and devices. The simulation framework validation relies on the comparison with measurements obtained under similar conditions, and it has been proved up to fluences of $\sim 10^{16}$ $\mathrm{n}_{eq}/\mathrm{cm}^2$. The already developed numerical models for the radiation damage effects must be extended to the extreme fluences accounting for the modeling of dopant removal, impact ionization, carriers' mobility and lifetime, and trap dynamics. As numerical simulations validate experimental results, they gain predictive capabilities, thereby reducing time

Table 1: Details of the EVL radiation damage modeling scheme.

	Acceptor	**Donor**
Energy [eV]	$E_C - 0.525$	$E_V + 0.48$
η **[cm^{-1}]**	0.03	0.08
σ_e **[cm^2]**	1.0×10^{-15}	$> 6.0 \times 10^{-16}$
σ_h **[cm^2]**	1.0×10^{-15}	5.5×10^{-15}

Table 2: Details of the LHCb radiation damage modeling scheme.

	Acceptor	**Acceptor**	**Donor**
Energy [eV]	$E_V + 0.90$	$E_C - 0.525$	$E_V + 0.48$
η **[cm^{-1}]**	36	0.75	4
σ_e **[cm^2]**	1.0×10^{-16}	5.0×10^{-15}	2.0×10^{-14}
σ_h **[cm^2]**	1.0×10^{-16}	1.0×10^{-14}	1.0×10^{-14}

and cost in detector design, development, and optimization before the actual manufacturing process. This promotes the development of new detector technologies.

3.1 EVL model

The *EVL model* (Table 1) provided by Eremin et al. [4] is capable of reproducing the double junction/double peak effect of the electric field in irradiated devices [5]. It considers both types of deep-level defects: a single donor defect in the lower half and a single acceptor level in the upper half of the silicon bandgap. When highly irradiated detectors are fully depleted ($V > V_{FD}$), a double peak transient current response appears, evincing the non-regular electric field distribution in the detector bulk with peaks near both contacts.

Eber et al. [6] have demonstrated that achieving agreement with measured I-V curves, and to some extent, Charge Collection Efficiency (CCE) up to a fluence of 1×10^{15} 1MeV n_{eq}/cm^2, is possible by incorporating only two energy levels. Additionally, these levels have been integrated with surface defects to simulate surface effects, as shown by Peltola et al. [7].

3.2 LHCb model

Building upon the existing model, an additional deep level was incorporated to enhance the reproduction of charge collection efficiency. This addition supplements the EVL model with the introduction of a third defect, and it is known as the *LHCb model* [8]. Table 2 summarises the parameters of the developed model using Synopsys Sentaurus TCAD.

The model assumes that defect state concentrations scale linearly with 1 MeV neutron equivalent fluence with a proportionality factor (introduction rate) η. The cross-sections and introduction rates of the two EVL levels were tuned to reproduce the measured I-V curve of the n-on-p reference pixel sensors. A shallow acceptor close to the conduction band was introduced, and its parameterization was tuned to reproduce the measured CCE of the reference sensors. This shallow acceptor has only a minor influence on the current generation and space charge, so it allows for tuning the CCE independently of the behavior of the I-V curves. Varying the hole capture cross-section within reasonable limits has a negligible effect on the CCE since the probability of hole capture is already very low due to the large distance from the valence band. To limit the number of degrees of freedom when scanning the parameter space, σ_h was chosen to have the same value as the electron capture cross-section. The physics models include Fermi-statistics, avalanche multiplication (Van Overstraeten–De Man model), the Slotboom model for the band gap narrowing, high field mobility saturation, Shockley–Read–Hall generation–recombination for the traps, and the Hurkx model for the trap assisted tunneling. The drift-diffusion model has been used, implying that the temperature of

Table 3: Details of the Delhi-2014 bulk damage modeling scheme.

	Acceptor	**Donor**
Energy [eV]	$E_C - 0.51$	$E_V + 0.48$
η **[cm^{-1}]**	4	3
σ_e **[cm^2]**	2.0×10^{-14}	2.0×10^{-14}
σ_h **[cm^2]**	2.6×10^{-14}	2.0×10^{-14}

Table 4: Details of the Delhi-2014 interface damage modeling scheme.

Trap type	**Energy [eV]**	η **[cm^{-1}]**	σ_e **[cm^2]**	σ_h **[cm^2]**
Acceptor	E_C-0.60	$0.6 \cdot N_{OX}$	$1.0 \cdot 10^{-15}$	$1.0 \cdot 10^{-15}$
Acceptor	E_C-0.39	$0.4 \cdot N_{OX}$	$1.0 \cdot 10^{-15}$	$1.0 \cdot 10^{-15}$
	Fluence [n$_{eq}$/cm^2]	**Concentration [cm^{-3}]**		
Oxide charge	non-irradiated	$5.0 \times 10^{10} - 5.0 \times 10^{11}$		
	1.0×10^{14}	$1.0 \times 10^{11} - 8.0 \times 10^{11}$		
	5.0×10^{14}	$5.0 \times 10^{11} - 1.2 \times 10^{12}$		
	1.0×10^{15}	$8.0 \times 10^{11} - 2.0 \times 10^{12}$		

the whole device remains constant. It has demonstrated good agreement with the I-Vs of irradiated 3D detectors but overestimated the breakdown voltage (V_{BD}) [9].

3.3 Delhi-2014 model

The *Delhi-2014* modeling scheme has been developed for 23 MeV proton irradiation using Silvaco TCAD [10]. The bulk damage is described with two trap levels which can reproduce the double-peak electric field. In addition, fixed oxide charge densities (N$_{OX}$) and interface traps (N$_{IT}$) at the silicon-oxide interface are taken into account. The N$_{OX}$ is described through a look-up table as a function of fluence while the N$_{IT}$ has been modeled with two acceptor traps with concentrations dependent on the N$_{OX}$ and with identical capture cross-sections independent of the type if σ_e or σ_h. The complete modeling scheme is reported in Table 3 and Table 4.

3.4 Hamburg Penta Trap Model

The *Hamburg Penta Trap Model* (HPTM) relies on a 5-level trap parameterization for the bulk radiation damage effects. It has been developed using the optimizer tool of Synopsys Sentaurus TCAD (Tab. 5). The trap types and their energy levels were derived from microscopic measurements. Their characteristics (η, σ_e and σ_h) were fine-tuned to reproduce the electrical behavior of p-type pad diodes irradiated with protons in the fluence range from 3×10^{14} n$_{eq}$/cm^2 to 1.3×10^{16} n$_{eq}$/cm^2. The optimizer tool utilized three free parameters for each trap, aiming to minimize the relative deviation between simulations and measurements across an extensive voltage range in terms of I-V, C-V, and CCE measurement sets. The impact ionization model considered is the van

Trap type	**Energy [eV]**	η **[cm^{-1}]**	σ_e **[cm^2]**	σ_h **[cm^2]**
Acceptor	$E_C - 0.458$	0.6447	2.551×10^{-14}	1.511×10^{-13}
Acceptor	$E_C - 0.545$	0.4335	4.478×10^{-15}	6.709×10^{-15}
Donor	$E_C - 0.1$	0.0497	2.300×10^{-14}	2.920×10^{-16}
Donor	$E_V + 0.48$	0.5978	4.166×10^{-15}	1.965×10^{-16}
Donor	$E_V + 0.36$	0.3780	3.230×10^{-17}	2.036×10^{-14}

Table 5: Details of the HPTM damage modeling scheme.

Table 6: Details of the *Perugia 2019 Surface* damage modeling scheme.

	Acceptor band	**Donor band**
Energy [eV]	$E_C - 0.56 \le E_T \le E_C$	$E_V \le E_T \le E_V + 0.60$
Width [eV]	0.56	0.60
$\mathbf{D}_{IT}$ **[eV^{-1}cm^{-2}]**	$D_{ITacc}(\phi)$	$D_{ITdon}(\phi)$
$\mathbf{N}_{IT}$ **[cm^{-2}]**	$N_{ITacc}(0) + \Delta N_{ITacc}(\phi)$	$N_{ITdon}(0) + \Delta N_{ITdon}(\phi)$
σ_e **[cm^2]**	1.0×10^{-16}	1.0×10^{-15}
σ_h **[cm^2]**	1.0×10^{-15}	1.0×10^{-16}
	Fixed oxide charge	
$\mathbf{Q}_{OX}[cm^{-2}]$	$Q_{OX}(0) + \Delta Q_{OX}(\phi)$	

Table 7: Details of the *New Univ. of Perugia* bulk damage modeling scheme.

	Acceptor	**Acceptor**	**Donor**
Energy [eV]	$E_C - 0.42$	$E_C - 0.46$	$E_C - 0.23$
η **[cm^{-1}]**	1.6	0.9	0.006
σ_e **[cm^2]**	1.0×10^{-15}	7.0×10^{-14}	2.3×10^{-14}
σ_h **[cm^2]**	1.0×10^{-14}	7.0×10^{-13}	2.3×10^{-15}

Overstraeten-de Man. For the acceptor defect at $E_C - 0.545$ eV, which is located close to midgap, the trap-assisted tunneling model from Hurkx with a tunnel mass of 0.25 m_e is used. Further details are provided in [11].

3.5 New University of Perugia model

Within a hierarchical approach, increasingly complex models have been considered, aiming at balancing complexity and comprehensiveness [12]. An enhanced modeling scheme, yet physically based, was eventually developed, featuring three dominant deep-level recombination centers (two acceptors and one donor). The model was capable of reproducing all the main evidence related to the radiation damage effects, namely the double-sided depletion effect, the depletion voltage values, the increase of the leakage current with fluence, and the charge collection efficiency trend with increased fluences [13].

Recently, the *New University of Perugia* comprehensive numerical modeling scheme that accounts for the combined effect of surface and bulk radiation damage on silicon detectors has been updated. The model has been developed and it is fully implemented within the Synopsys Sentaurus TCAD environment. At the development stage, a physics-driven approach has been pursued to keep the number of fitting parameters as low as possible, thus devising a not overspecific modeling scheme.

Surface damage significantly impacts the surface generation current, the breakdown voltage, the inter-electrode isolation, and the capacitance, and may affect the charge collection properties of solid-state sensors. For TCAD simulation purposes, the surface radiation damage effects can be ascribed to the building up of trapped charge within the oxide (Q_{OX}) and the increase in the number of interface trap states (N_{IT}). The *Perugia 2019 Surface* damage model considers two bands of defects, one acceptor and one donor (Table 6), and their parameterization is detailed in [14, 15]. N_{IT} and N_{OX} were determined before and after X-ray irradiation with doses up to 100 Mrad (SiO_2) from test structures exploring various design options, diverse vendors, and technology alternatives. The surface radiation damage model can be combined with the effect of displacement damage (bulk damage), accounting for silicon lattice defect generation and point and cluster defects in terms of the increase of bulk deep-level trap states for the analysis of more complex structures [16]. The *New University of Perugia* bulk model relies on three defect levels, two acceptors and one donor, as detailed in Table 7. It has been extensively applied to the study of PiN diodes, LGAD-based detectors (compensated LGAD, AC-RSD, and DC-RSD) [17, 18], where it has been coupled to the acceptor removal mechanism of the gain layer and the acceptor creation of the bulk based on the *Torino parameterization* [19]. The acceptor-removal mechanism in the multiplication layer follows the analytical law for the concentration $N_{GL}(\phi) = N_A(0)\exp^{-c\phi}$, where N_{GL} is the peak dose of the gain-layer profile, ϕ is the fluence, $N_A(0)$ is the initial acceptor density and c is a constant. In addition, the acceptor creation at the bulk level follows:

$$N_{A,bulk} = \begin{cases} \mathrm{N}_{A,bulk}(0) + g_c\phi & 0<\phi \leq 3\times 10^{15}\ n_{eq}/cm^2 \\ 4.17{\times}10^{13}\cdot ln(\phi) - 1.41\times 10^{15} & \phi > 3\times 10^{15}\ n_{eq}/cm^2 \end{cases} \tag{1}$$

where $g_c = 0.0237\ \mathrm{cm}^{-1}$.

4. Conclusion

Various TCAD models for the description of radiation damage effects consider different numbers of defects with distinct parameters. This implies that there is not a unique parameterization, and multiple models may be effective.

While TCAD simulation is a robust tool for studying silicon detectors, it is crucial to compare measurements with simulations to refine models and trap parameterization. Presently, achieving a simulation modeling scheme capable of effectively describing the entire range of measurements for radiation damage remains a challenge. There is a pressing need to develop a versatile model applicable to various detectors and irradiation levels. This would facilitate a better understanding of the behavior of novel detectors and support design optimization efforts.

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