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TCAD and charge transport simulations of MAPS in 65 nm for the ALICE ITS3

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Abstract: As part of the upgrade to the Inner Tracking System 3 (ITS3) for ALICE and the strategic R&D programme of the CERN EP department, stitched Monolithic Active Pixel Sensors (MAPS) are being developed using a 65 nm CMOS imaging process. Several sensor prototypes were characterized in laboratory using radioactive sources, particularly the ^{55}Fe source, which was extensively used. The analysis of the resulting spectra provided valuable insights into the charge collection performance of these sensors, which were critical for validating the sensor design and its suitability for ITS3. To gain a deeper understanding of the behavior of the sensors, simulating the charge transport mechanisms within these sensors is essential. This study consists of simulating the electric field of the sensor using Sentaurus TCAD and then use it in a Monte Carlo simulation in Garfield++ to model the charge transport mechanism and collection process. The resulting charge collection information is used as input in a Python program to simulate the chip response to X-rays coming from the ^{55}Fe source. The simulated spectra were found to be well in agreement with the experimental data, confirming the validity of the model.

Keywords: Detector modelling and simulations II (electric fields, charge transport, multiplication and induction, pulse formation, electron emission, etc); Particle tracking detectors; Performance of High Energy Physics Detectors; Simulation methods and programs

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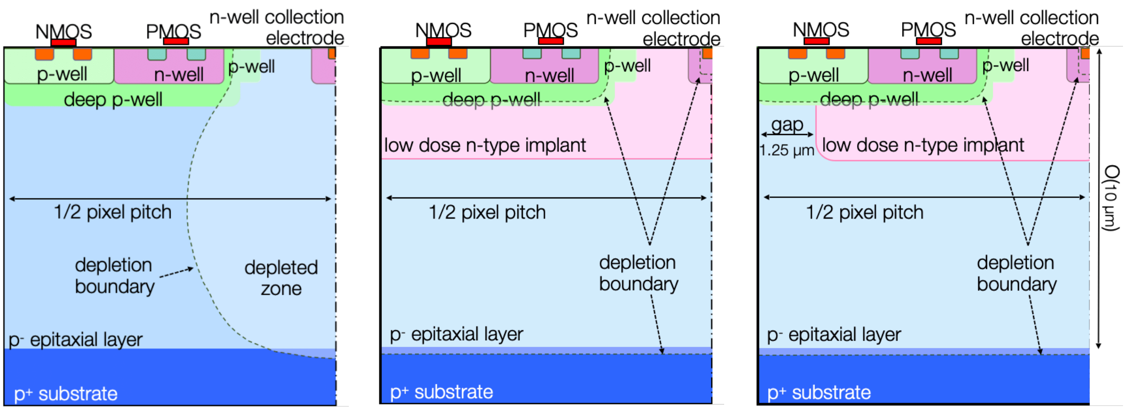
1 Introduction

The Inner Tracking System 3 (ITS3) is the new vertex detector proposed for the upgrade of the ALICE experiment at CERN planned for the LHC long shutdown 3. It will consist of bent, wafer-scale stitched monolithic pixel sensors manufactured in the TPSCo 65 nm CMOS imaging process [1], reducing the material budget to an average of $0.07\%X_0$ and the radius of the innermost layer to 19 mm. These advancements will improve the impact parameter resolution and tracking efficiency [2].

The development of MAPS in a 65 nm CMOS imaging process is a joint effort with the strategic R&D programme of the CERN Experimental Physics (EP) department. To validate this technology for High Energy Physics (HEP), many test structures were designed and tested. In particular the Analogue Pixel Test Structure (APTS) was extensively characterised with an ^{55}Fe source to study the charge collection performance of different variants [3].

The pixel sensor design consists of a small n-well collection electrode and a high-resistivity p-type epitaxial layer grown on p-type substrate, with the in-pixel circuitry located in deep p-wells. A negative bias (back-bias) can be supplied both to the substrate and to the deep p-wells. Three different sensor designs (shown in figure 1) were implemented as APTS variants to test their charge collection



(a) Standard process. (b) Modified process. (c) Modified with gap process.

Figure 1. Half cross-sections of the three different pixel designs implemented: (a) standard: no additional low-dose implant, (b) modified: with deep blanket low dose n-type implant, and (c) modified with gap: with a gap in the deep low dose n-type implant at the pixel borders. Reproduced from [3]. CC BY 4.0.

performance: the standard design, without a deep low-dose n-type implant, where the epitaxial layer is typically not fully depleted and the charge generated outside the depletion region is collected primarily by diffusion, the modified design, with a deep low-dose n-type implant under the full pixel area that allows full depletion of the epitaxial layer and a faster charge collection by drift, and the modified with gap design, where the same low dose n-type implant features a gap of 2.5 µm (1.25 µm per side) at the pixel boundaries. This gap prevents low-field regions on the boundary between pixels and creates a vertical junction to increase the lateral electric field pushing the charge from the pixel boundary towards the collection electrode, thus reducing the charge sharing among neighbouring pixels [4].

2 Simulation workflow

The goal of this study is to reproduce the ^{55}Fe spectrum (K_α X-ray: energy of 5.9 keV and probability of 28%, K_β X-ray: energy of 6.49 keV and probability of 2.9%) simulating the charge collection process in the sensor and its response to X-rays. The structure of the simulation workflow is illustrated in figure 2. The first phase consists of using a TCAD (Technology Computer-Aided Design) [5] simulation to extract the electric field of a single pixel cell of the sensor. This simulation step requires as input the doping profiles and geometry parameters of the sensor, which collectively influence the electric field distribution within the pixel.

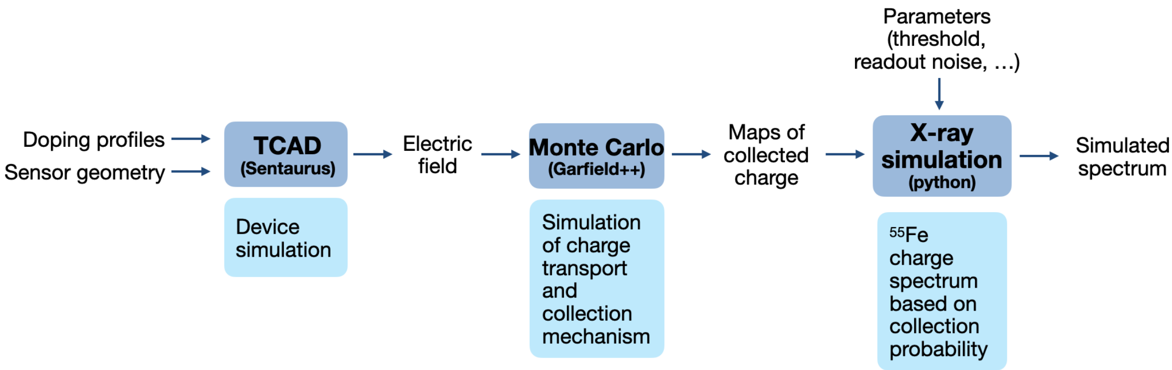


Figure 2. Sketch of the simulation workflow.

Following this, the electric field data serves as input to the Monte Carlo simulation in Garfield++, a specialized simulation designed to model charge transport and collection processes within the sensor [6]. In this phase, a fixed number of electrons is systematically injected into the central pixel of a 5×5 matrix and propagated through a Monte Carlo-based integration in Garfield++ until they either recombine or reach one of the collection electrodes of the matrix.[1] The distribution of the final states of electrons is saved and later, by sampling from this distribution, the final state of an electron starting at the same position can easily be estimated. This injection is performed at various positions scanning the full device in all dimensions. The purpose of this step is to produce a set of charge collection maps, linking each starting position in the sensor to the amount of charge collected at each pixel within the matrix.

In the final step, these charge maps are used to model the response of the chip to X-rays, specifically from the ^{55}Fe source. The ^{55}Fe spectrum has been chosen as a reference for its characteristic shape

[1]No formulation of induced charge is included, as only the integrated charge is taken into consideration.

that demands precise modelling for alignment with experimental data. In this phase, different X-ray energies are simulated separately, accounting for charge spread (modelled using the Fano factor), attenuation length, and photon counts, and then combined to reflect the total sensor response.

The factorization of the full simulation into three parts is done to isolate the computationally intensive and doping dependant Garfield++ simulation in such a way that the generated maps can be easily reused for simulations involving different particles and conditions.

3 Lifetime implementation

Simulation results and experimental data were first compared for a modified with gap APTS with a 15 µm pixel pitch. Initial results showed good alignment in the main peaks of the measured and simulated spectra but revealed discrepancies in the lower charge region (below 800 electrons), as shown in figure 3(a). Additionally, the cluster size distributions showed a mismatch in charge-sharing behavior, particularly in the ratio of events with cluster sizes of 1 and 2, as shown in figure 3(b). These differences could be attributed to carriers originating from the substrate, suggesting that the simulation model may inaccurately represent substrate effects, like recombination. To address this, the carrier lifetime modelling approach was analyzed in detail, as accurate modelling of recombination is crucial for reflecting substrate impact on charge collection.

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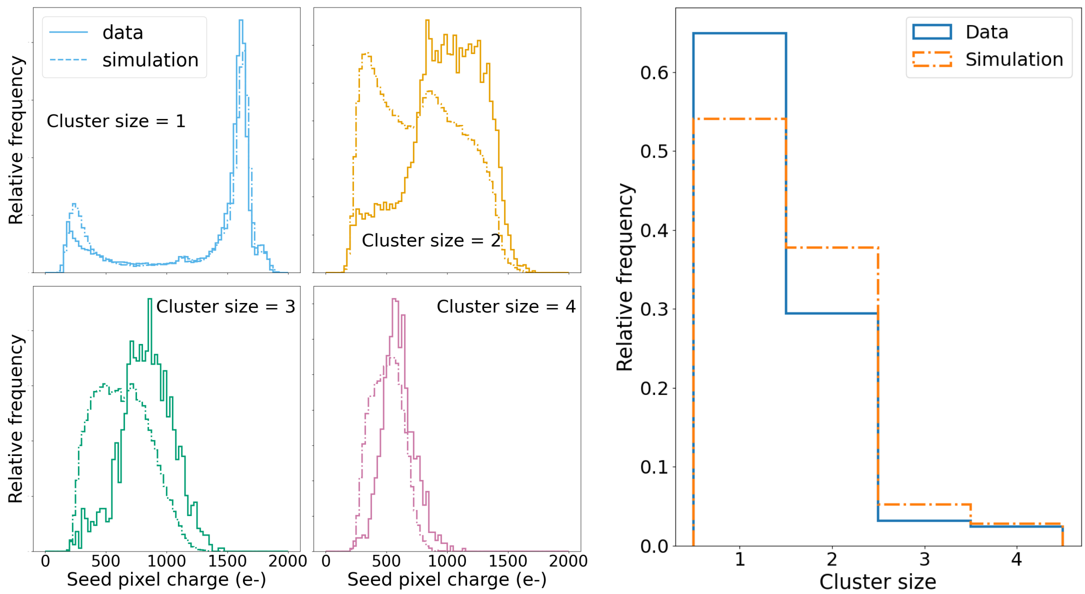


(a) ^{55}Fe spectra for different cluster sizes.

(b) Cluster size distributions.

Figure 3. Comparison between (a) simulated and measured ^{55}Fe spectra for different cluster sizes, and (b) simulated and measured cluster size distributions. Each sub-plot is normalised individually. Simulations carried out without a recombination model in Garfield++. These data refer to a modified with gap APTS with a pixel pitch of 15 µm and at a back-bias of 1.2 V.

At the onset of this simulation study, the standard version of Garfield++ did not yet provide a carrier lifetime implementation compatible with the TCAD import, nor a recombination modelling for very low electric field regions. The recombination effect model has been extended to support these scenarios and integrated in an upgraded version of the Garfield++ framework.

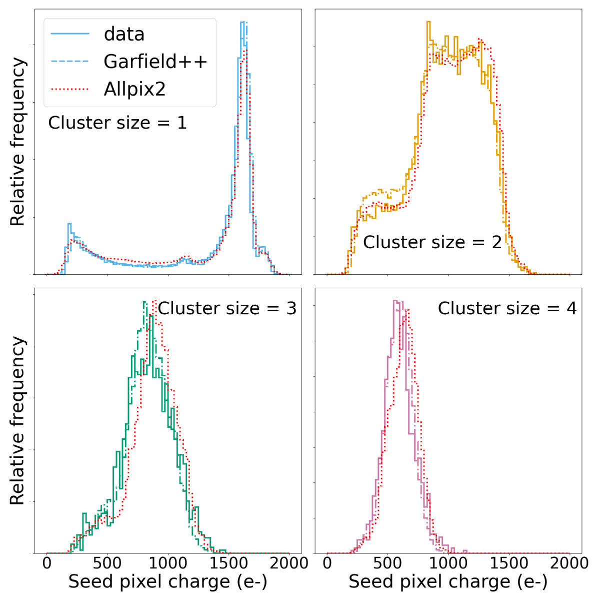
TCAD simulations provide detailed spatial distributions of parameters like the minority carrier lifetime, and mobility. These distributions reflect variations in doping concentration and electric fields. By importing the output of TCAD simulations into the Garfield++ framework, it becomes possible to accurately simulate charge transport and recombination effects.

This upgraded version of Garfield++ incorporates recombination probability maps derived from TCAD simulations, which are imported into Garfield++ as spatially dependent tables. During each transport step, the framework evaluates the recombination probability based on the spatial position of the carrier.

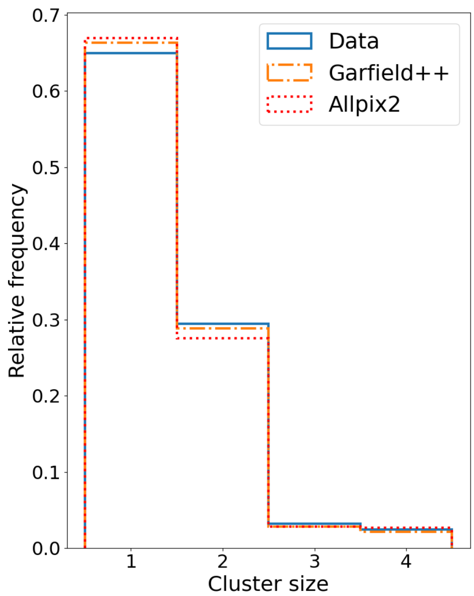
4 Results

The results of this implementation are presented in figure 4(a) and figure 4(b), for charge sharing and cluster size distributions, respectively. These plots demonstrate a much better agreement between simulation and experimental data, with only minor discrepancies observed.

Similar simulations were also carried out, producing the maps of the collected charge with Allpix squared, a well-established software framework for silicon detectors [7], essentially producing similar results.



(a) ^{55}Fe spectra for different cluster sizes.



(b) Cluster size distributions.

Figure 4. Comparison between (a) simulated and measured ^{55}Fe spectra for different cluster sizes, and (b) simulated and measured cluster size distributions. Each sub-plot is normalised individually. Simulations carried out with the new recombination modelling of Garfield++ and Allpix squared framework. These data refer to a modified with gap APTS with a pixel pitch of 15 µm and at a back-bias of 1.2 V.

Another important confirmation of the accuracy of the model lies in its ability to simulate the standard design, where the diffusion mechanism dominates over the drift due to the presence of a partially depleted region (see figure 1(a)). Figure 5 depicts the simulated spectra of all the APTS sensor design variants shown in figure 1. These results demonstrate that the model effectively captures

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the carrier dynamics, providing an accurate representation even in regions where diffusion has a significant influence on carrier lifetime.

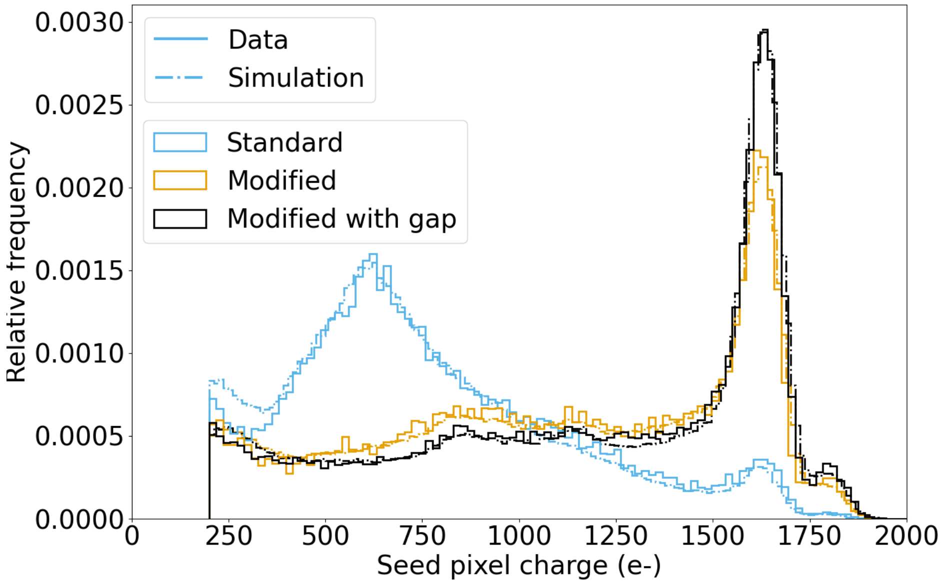

Figure 5. Comparison between simulated and measured ^{55}Fe spectra for different implant geometries. Simulations carried out with the new recombination modelling of Garfield++. These data refer to APTS pixel pitch of 15 µm and at a back-bias of 1.2 V.

5 Conclusions

The simulation studies on a 65 nm CMOS imaging process prototype advanced the understanding and modelling of their performance. A simulation workflow was developed, integrating TCAD simulations for electric field modelling, Garfield++ for charge transport, and a Python framework for X-ray interactions and sensor response. Simulated and experimental spectra show excellent agreement, validating the framework, though discrepancies in the low-charge region highlighted the need to model recombination and charge transport effects accurately. Direct implementation of these effects in Garfield++ improved simulation accuracy. This versatile simulation framework is now capable of accommodating multiple chip variants and conditions. These advancements not only provide valuable insights into the behavior of APTS chips but also establish a robust foundation for future studies. The next major milestone will be to accurately simulate the effects of irradiation on these sensors.

Acknowledgments

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