PROCEEDINGS OF SCIENCE

Modeling radiation damage in TCAD

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The aim of this work is to develop a TCAD radiation damage model at a device level, enabling a predictive insight on the electrical behaviour of detectors and aiming at their ultimate performance optimization for the operation at HL-LHC expected fluences (e.g. greater than 2.0×10^{16} 1 MeV equivalent neutrons/cm^2). Our approach aims at keeping the number of fitting parameters as low as possible, at the same time accounting for new experimental evidences of relevant effects at these very high fluences (e.g. charge multiplication and avalanche effects). A physically grounded approach is being pursued, aiming at devising a not over-specific modelling while keeping predictive capabilities on the device behavior fabricated by different vendors (e.g. with different technology flavors) and in different operating conditions, e.g. at different fluences, temperatures and biasing voltages. The model development follows a test campaign with a twofold goal: from one hand, the relevant technology parameters such as oxide charge and interface trap states as a function of the irradiation dose have been measured. On the other hand, DC and AC measurements on gate-controlled diodes and MOS capacitors can be used as reference for TCAD simulation models validation purpose. The complete bulk and surface radiation damage model can be exploited for the analysis of the active behavior of different classes of new generation detectors to be used in the future HEP experiments.

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1. Introduction

Modern Technology CAD (TCAD) tools offer a wide variety of approaches for the analysis and simulation of semiconductor devices, characterized by different combinations among physical accuracy and comprehensiveness, application versatility and computational demand. Mixed-mode (e.g. device/circuit level) simulation approaches can be efficiently followed in order to predict the electrical behavior of solid-state detectors in different operating conditions. In particular, radiation hardness is a critical design constraint for current and future generation silicon detectors, which are expected to undergo extremely high fluences (e.g. greater than 2.0×10^{16} 1 MeV equivalent neutrons/cm^2). Within the detector operating life, progressive radiation damage is hence to be properly taken into account: a number of different physical damage mechanisms actually may interact in a non-trivial way. Deep understanding of physical device behavior therefore has the utmost importance, and device analysis tools may help to this purpose. In this work, bulk and surface radiation damage have been taken into account by means of the introduction of deep level radiation induced traps whose parameters are physically meaningful and whose experimental characterization is feasible. Within a hierarchical approach, increasingly complex models have been considered, aiming at balancing complexity and comprehensiveness.

Different TCAD modeling approaches have been developed and applied in the past in order to predict the behavior of progressively irradiated device. Extending the original work of [1], [2] a multiple deep-levels model has been proposed by Pennicard et al. in [3]. Three levels have been used, by increasing their defect capture cross-sections in order to emulate the inter-defect coupling responsible of the increased leakage current with respect to what foreseen by a classical SRH statistics. Verbitskaya et al. [4] proposed a simplified model based on one acceptor and one donor level, accounting for avalanche multiplication effects at the same time relying on a mono-dimensional analytical approach. On the other hand, a more articulated picture in terms of bandgap modelling has been proposed by Dalal et al. [5], including up to five deep-level traps and separated effects of oxide and interface trapped charge. Within the CERN RD50 collaborations, a lot of work is being carried out, as summarized in e.g. [6]. A 3-level model for bulk, combined with a thin (2 μm depth) layer for surface effects has been considered, along with different modeling parametrization for neutron and proton irradiation. A more recent approach has been proposed by the Hamburg group following a global optimization based on multiple fitting parameters [7].

2. Combined surface and bulk TCAD modelling

The variety of the approaches described in the previous section points out the complexity of the problem of devising a reliable, as well as suitable for provisional analysis model accounting in a comprehensive way the radiation damage effects. The aim of this work is to extend the predictive capabilities of the previous Perugia model [1], [2] up to radiation damage levels expected at HL-LHC (e.g. greater than 2.0×10^{16} 1 MeV equivalent neutrons/cm^2). Our approach aims at keeping the number of fitting parameters as low as possible, at the same time accounting for new experimental evidences of relevant effects at these very high fluences (e.g. charge multiplication and avalanche effects). A physically grounded approach is still being pursued, aiming at devising a not over-specific modelling while keeping predictive capabilities on the device behavior fabricated

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by different vendors (e.g. with different technology flavors) and in different operating conditions, e.g. at different fluences, temperatures and biasing voltages. It is worthwhile to stress that the goal of this approach is not to model the complex phenomenology of the radiation damage mechanisms at atomistic level. Instead, our primary concern is the modelling the *effects* of the radiation damage at a device level, enabling a predictive insight on the electrical behaviour of detectors and aiming at their ultimate performance optimization. Within this framework, radiation damage effects can be summarized in two main classes: ionizing and non-ionizing effects. Ionizing effects can be ascribed to surface damage (or interface damage), namely the build-up of trapped charge in the oxide, the increase in the number of bulk oxide traps and the increase in the number of interface traps. For TCAD simulation purposes, such effects can be described in terms of fixed oxide charge (Q_{OX}) and interface trap states densities (N_{IT}). On the other hand, non-ionizing effects can be ascribed to a bulk damage: silicon lattice defect generations, point and cluster defects formation and therefore an increase of deep-level trap states. Traps provide allowed energy states within the semiconductor band-gap, affecting the device behavior to many respects, e.g. by altering the effective doping, by enhancing recombination and by increasing leakage current. From TCAD stand-point, several models, e.g. Shockley-Read-Hall recombination, depend on traps implicitly. The correct trap parametrization is therefore of utmost importance in order to correctly describe the radiation damage effects. With reference to the state-of-the-art Synopsys Sentaurus TCAD tool, traps have to be described by defining their type (acceptor or donor), energy distribution (Level, Gaussian, Uniform, ...), capture cross-sections for both electrons and holes and concentration / spatial distribution. In particular, acceptor traps are uncharged when unoccupied (empty) or negatively charged when occupied (they carry the charge of one electron when fully occupied). On the other hand, donor traps are uncharged when unoccupied (empty) or positively charged when occupied (they carry the charge of one hole when fully occupied). Even if traps located in the upper half of the band gap energy are usually assumed as acceptor and traps located in the lower half are assumed as donor, the trap type definition should be therefore carefully taken into account, in particular when describing interface trap states which typically act as amphoteric traps.

3. TCAD radiation damage model parametrization and validation

An intensive measurement campaign on both non-irradiated and irradiated test structures has been carried out, as described in [9], [11]. The aim of this test campaign was twofold: from one hand, the relevant technology parameters such as oxide charge and interface trap states as a function of the irradiation dose have been measured. On the other hand, DC and AC measurements on gate-controlled diodes and MOS capacitors can be used as reference for TCAD simulation models validation purposes. Standard C-V measurements at high and low frequencies of MOS capacitors fabricated on both *n*-type and *p*-type substrates have been carried out in order to extract the relevant parameters to be used in the simulations. As an example, the effective oxide charge density increase (i.e. the equivalent oxide charge increase responsible for the flat-band voltage shift) due to both fixed oxide charge increase as well as interface trap state density increase with irradiation dose is reported in Fig. 1. Following the measurement procedure described in [11] and the method proposed by [12] it is actually possible to separately evaluate the effect of oxide charge and interface traps increase with dose. This information can be therefore fed into the simulator and, e.g., small-signal analyses can be carried out. The acceptor interface trap states density as measured from *n*-type substrates test structures is reported in Fig. 2. In this case, it can be pointed out that a non-negligible acceptor-like trap states is to be considered close to the conduction band edge. Similar measurements have been carried out on *p*-type substrates for donor interface trap state evaluation purposes, showing a less significant donor trap concentration close to the valence band.

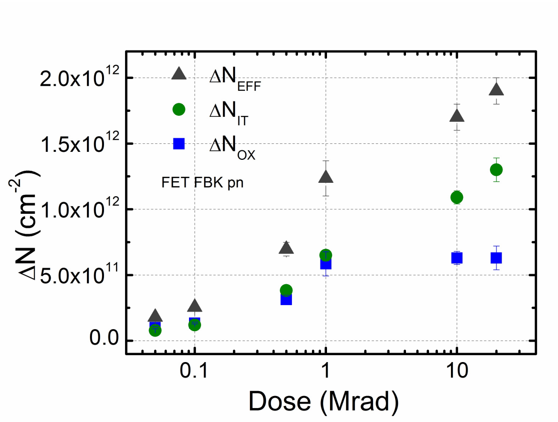


Figure 1: Measured effective oxide charge contributions as a function of the irradiation dose.

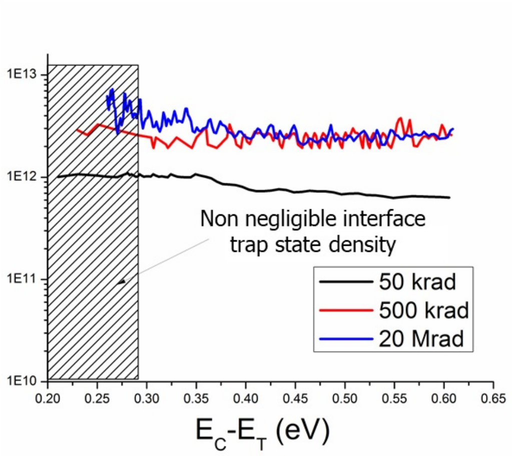


Figure 2: Measured acceptor interface trap states spectral density.

For simulation purposes, to begin with, a simplified structure has been considered, featuring a simple one-strip like n-on-p junction (Fig. 3). The effect of different capture cross sections of a deep-acceptor bulk trap level (E_a = E_c - 0.46 eV) on the leakage current have been evaluated. Only marginal effects on steady-state I-V curves can be appreciated, at least within a reasonable variation range of the capture cross-sections (e.g. smaller than 1.0×10^{13} cm^{-2}). On the other hand, the effect of the impact ionization (avalanche generation) is significant at these very high fluences, greatly reducing the breakdown voltage (Fig. 4).

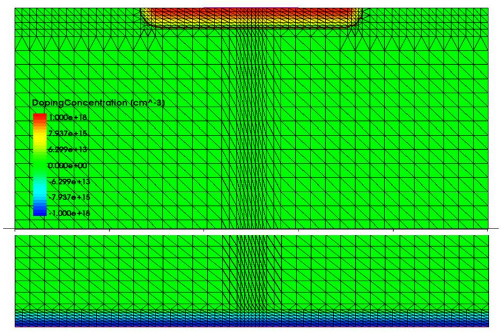


Figure 3: Sketch of the simulated one strip-like structure.

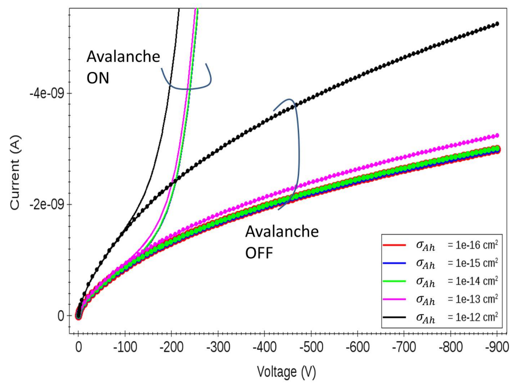


Figure 4: I-V curves for different bulk acceptor cross-sections.

Slightly more complicated test structures such as gate controlled diodes (Fig. 5) can be used to evaluate the effects of interface trap parametrization. In particular, I-V curves extracted from gate controlled diodes can be used in order to cross-check the surface recombination velocity as extracted from measurements with experimental findings (Fig. 6). The good agreement between measurements and simulation allows the validation of the modeling approach ([8], [10]).

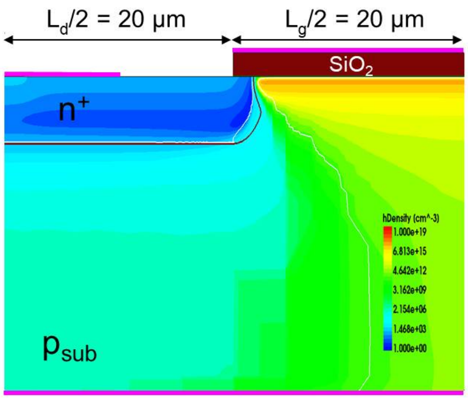


Figure 5: Sketch of the simulated gated diode sub-section structure.

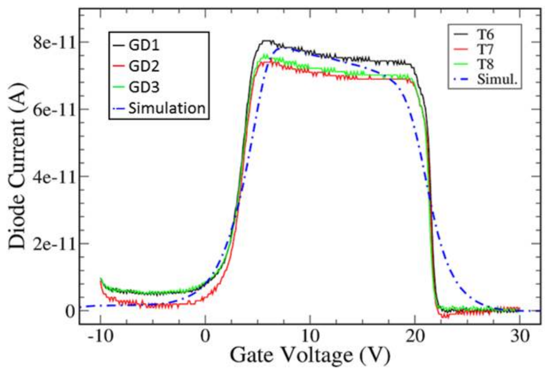
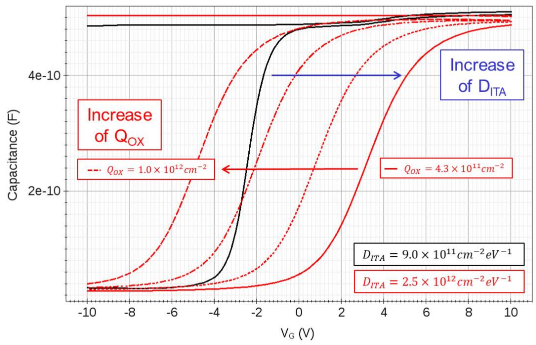


Figure 6: I-V gated diode currents: measurements vs. simulations.

A parametric analysis has been carried out, aiming at evaluated the model parametric sensitivity, e.g. in terms of the flat-band voltage shift with respect to acceptor interface trap state (*n*-type substrate), and oxide charge (Fig. 7). As expected, the increase of the (positive) oxide charge causes a left shift of the C-V high-frequency curves, while the increase of the acceptor trap states, acting as electrons (negative charges) trap has the opposite effect.



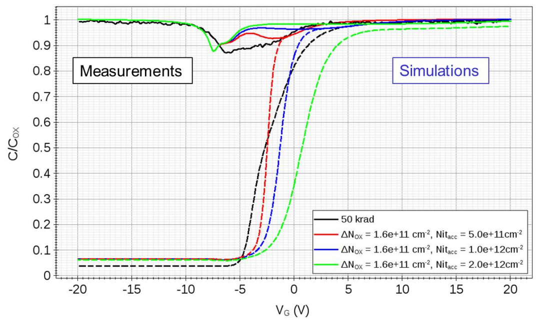


Figure 7: Sensitivity analysis: effect of oxide charge and interface acceptor trap density.

Figure 8: C-V measurements vs. simulations: High-Freq. dashed lines, Quasi-Stationary solid lines.

The model predictive capabilities for progressively irradiated devices can be investigated as well, enabling a comparison between simulations and measurements irradiated structures. Actually, using the oxide charge as fitting parameter the measured behavior of test structures at hand can be satisfactorily reproduced, as illustrated in Fig. 8 where quasi-stationary and high-frequency measurements on a irradiated MOS capacitors are reported, along with different simulated curves corresponding to different values of the oxide charge. In the figure, black curves represent the measurements, while colored lines represent simulations related to different oxide charge values.

Eventually, the complete bulk and surface radiation damage model can be exploited for the analysis of the active behavior of tracking detectors. As an example, microstrip detectors have been considered. In particular, the current responses to different particle impact locations of a 5-strips sub-section have been simulated, aiming at evaluating the charge collection efficiency for progressively irradiated structures. A summary comparison between simulations and measurements in terms of charge collection at different biasing voltages (T = 248 K) is reported in Fig. 10.

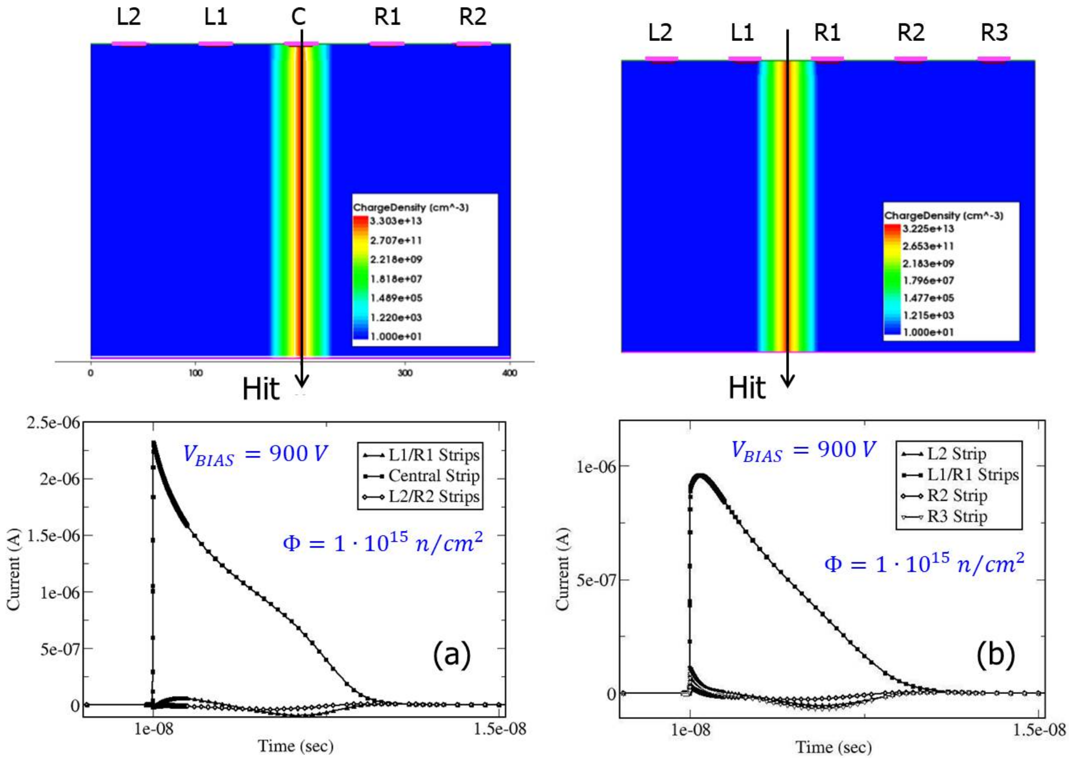


Figure 9: Current responses of a 5-strip structure to different hit positions (V_{BIAS} = 900V, Φ=1.0 $\times$ 10^{15} 1 MeV equivalent neutrons/cm^2).

4. Conclusion

TCAD modelling of radiation damage effects is definitely a tough task. In this work surface radiation damage effects have been deeply investigated aiming at the extraction of the most relevant parameters (oxide charge, interface trap states and trapped charge) to be used in simulations. The aim was the development of a comprehensive radiation damage modelling scheme, including bulk and surface effects suitable for commercial TCAD tools (e.g. Synopsys Sentaurus). The predictive capabilities of the new *University of Perugia* TCAD model have been extended to HL-LHC radiation damage levels, fostering its application to the analysis and optimization of different classes of detectors to be used in the future HEP experiments.

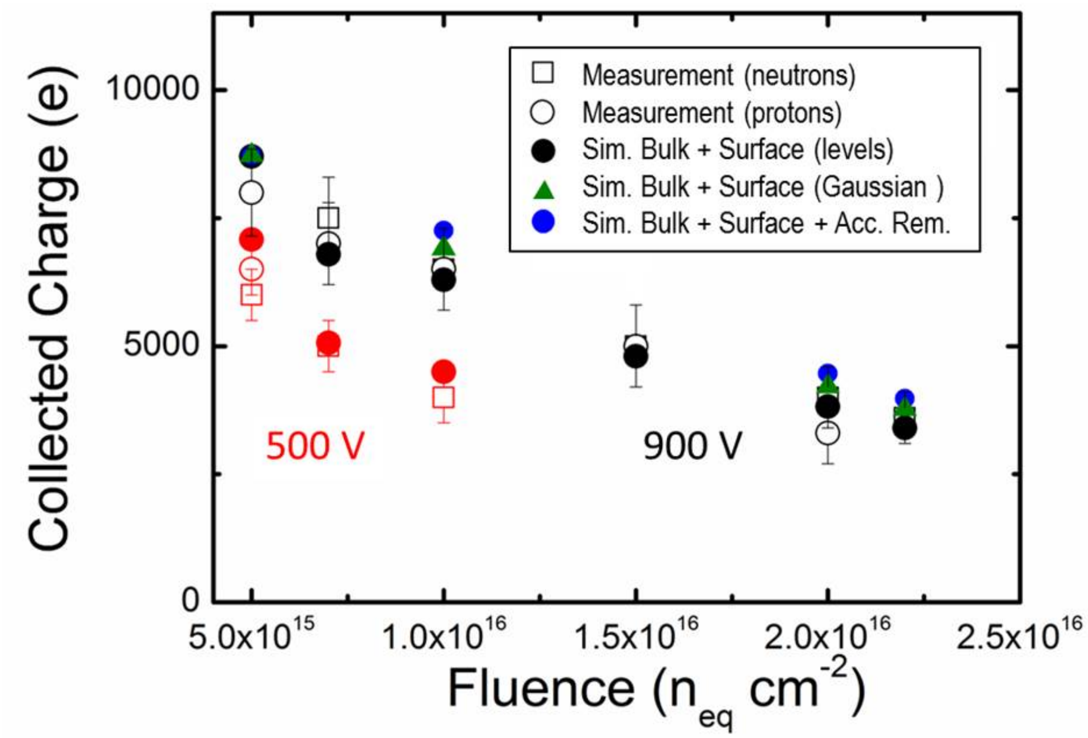


Figure 10: Charge collection as a function of fluence: simulations vs. measurements at different biasing voltages (measurements data from [13]).

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