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Abstract

The ion beam induced charge (IBIC) microscopy is a valuable tool for the analysis of the electronic properties of semiconductors. In this work, a recently developed Monte Carlo approach for the simulation of IBIC experiments is presented along with a self-standing software equipped with graphical user interface. The method is based on the probabilistic interpretation of the excess charge carrier continuity equations and it offers to the end-user the full control not only of the physical properties ruling the induced charge formation mechanism (i.e., mobility, lifetime, electrostatics, device's geometry), but also of the relevant experimental conditions (ionization profiles, beam dispersion, electronic noise) affecting the measurement of the IBIC pulses. Moreover, the software implements a novel model for the quantitative evaluation of the radiation damage effects on the charge collection efficiency degradation of ion-beam-irradiated devices. The reliability of the model implementation is then validated against a benchmark IBIC experiment.

Keywords stochastic approach, radiation damage, semiconductors modeling, microbeam, ion beam analysis

1. Introduction

In the last two decades the Ion Beam Induced Charge (IBIC) microscopy has been widely exploited to investigate the operation of semiconductor-based devices and microcircuits and to characterize the electronic properties of emerging materials [1,2]. Moreover, the technique has been used to study device- and material-related physical phenomena, such as single event [3], charge sharing [4,5] and radiation damage [6,7] effects in semiconductors and insulators. The IBIC technique is emerging as an ideal tool for radiation damage studies in semiconduting and insulating devices, as it offers the unique advantage of both monitoring the dose rate and the total implanted dose in selected regions of the sample [6], and simultaneously monitoring the charge collection efficiency (CCE) degradation as a function of the accumulated dose.

Moreover, the availability of a robust and reliable mathematical model based on the Shockley-Ramo-Gunn theorem [1,2,8,9] for the interpretation of the induced charge pulse formation allows an effective evaluation of the transport and electrostatic parameters for the electronic characterization of semiconductors. .

The theory and the computational model has been developed in the last decade and has been validated by benchmark experiments [2,8].

Recently, a new Monte Carlo approach has been developed to realistically model the induced charge pulse formation [10, 11] in order to include in the model variables following stochastic distributions, as statistical fluctuations in carrier generation, or randomly distributed recombination centres, electronic noise and thresholds.

To facilitate end users to simulate and interpret the experimental findings, a dedicated software, namely the IBIC Simulation Tool (IST) [12], offering a simple graphical user interface (GUI) has been recently developed.

Moreover, the IST is tailored to study, according to a recently proposed model [6], the radiation induced effects on the electronic properties of semiconductor and insulator devices.

In this paper, the main features of the Monte Carlo approach are discussed and validated against a benchmark experiment.

2. The Monte Carlo Approach

The Monte Carlo approach relies on the Shockley-Ramo-Gunn theorem [1,2,9], which states that the total induced charge q_j induced at the j-th electrode by a point charge q moving in a device with an arbitrary arrangement of electrodes and space charges can be evaluated as the difference in weighting potential between the initial and the final position of motion:

$$q_j = +q\left[\frac{\partial\psi(x_F)}{\partial V_j} - \frac{\partial\psi(x_I)}{\partial V_j}\right] \qquad (1)$$

where the weighting potential is defined as the derivative of the electric potential ψ with respect to the voltage V_j applied at the j-th electrode.

As a consequence, if the generation position x_I for an excess charge carrier q is known, the induced charge q_j can be determined through the simulation of a random walk, based on the carrier continuity equations [10]. Such a stochastic approach allows to simulate each ion strike as a package of N point-like electron-hole pairs (EHPs), generated according to the relevant ionization profile. The simulated CCE pulse for the particular probing ion is then given by the average value over the N independent simulations.

This method enables the full simulation of IBIC experiments. In fact, normally distributed random noise fluctuations can be added to each simulated IBIC pulse according to user-defined parameters, and a noise threshold filter can be applied to the set of resulting data. Moreover, an ion dispersion around the nominal position of incidence of the microbeam can be taken into account for the EHP generation profile. The process is then simulated over a set of independent ion hits, from which all relevant statistical parameters can be extracted. Finally, the nominal beam position can be swept over the whole beam scanning area to evaluate IBIC profiles and two-dimensional maps.

The Monte Carlo algorithm

The development of a comprehensive and self-consistent simulation software requires a reliable Monte Carlo kernel for the evaluation of the induced charge, and an application interfacing it with input/output data and user-defined parameters. A sketch of the IST operation workflow is represented in Fig. 1. The Monte Carlo method underlying the IST (details in [10]) is based on the finite difference form of the the excess carrier continuity equations. Considering a regular one-dimensional grid with constant space (Δx) and time (Δt) step, the holes equation can be it can be written as

$$p(x,t+\Delta t) = p(x,t)\cdot\left(-P_\tau(x)\right) + p(x+\Delta x,t)\cdot P_+(x) + + p(x-\Delta x,t)\cdot P_-(x,t) \qquad (2)$$

where the coefficients P_i are given by

$$P_\pm(x) = \frac{\Delta t}{(\Delta x)^2}D_p \mp \frac{\Delta t}{\Delta x}v_p \qquad (3)$$
$$P_\tau(x) = \frac{\Delta t}{\tau_p(x)}$$

In eq. (3), we assumed a linearized recombination term $1/\tau(x)$ under the assumption that the trapping center density is independent of the excess carrier concentration.

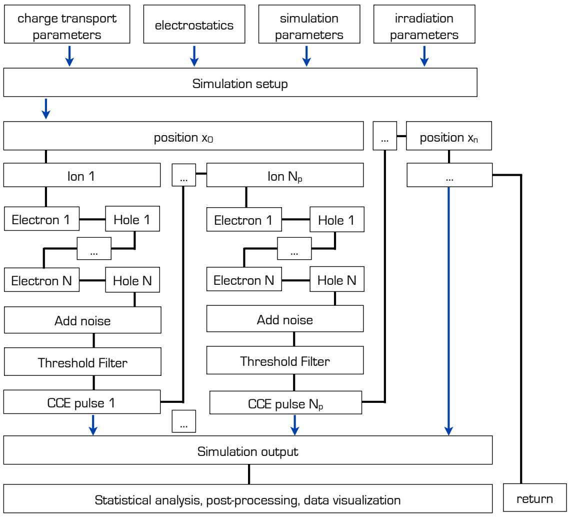

Fig. 1: Sketch of the IST operation workflow. User-defined parameters and profiles relevant to the simulation are set up by the initial step of the program. The first ion generation position x_0 is then chosen; N_p ions are there simulated as a package of N independent EHPs each. Each ion pulse is evaluated according to eqs. (1,2), and summed to pseudo-random noise fluctuations. The generation position is then swept along the device profile to reproduce a beam raster scan over the sample, and the simulation procedure is repeated. The simulation output consists of each simulated CCE pulse, along with its spatial coordinates and average time-resolved information. A real-time statistical data analysis is by the IST.

Defining $p(x\pm\Delta x,t)$ as the probability that at time t a hole can be found at position $x\pm\Delta x$, the coefficients $P_\mp(x)$ are then the relevant probabilities for the hole to be found at position x after a time interval Δt, respectively. Similarly, $P_\tau(x,t)$ represents the probability for the hole to recombine in the same interval. Therefore, eq. (2) defines a random walk, in which the coefficients (3) represent the drift-diffusion and recombination probabilities. Similar results can be obtained for electrons.

The isotropy of the carrier diffusion, i.e. $\Delta t = (\Delta x)^2/2D_p$, and the constraint on the probability coefficients $P_\pm \leq 1$, i.e. $\Delta x \leq 2D_p/v_{max}$, where v_{max} is the maximum drift velocity in the simulation domain, define the meshing conditions, for which the probabilistic interpretation is valid [10,11].

The electrostatic field and weighting potential profiles, required by eqs. (1,3) and defined on a regular mesh, are assumed as input data of the IST and can be imported from external files. Similarly, temperature, carrier lifetimes, saturation velocities and low field mobilities are regarded as user-defined parameters, which allow for the evaluation of the recombination probability profile $P_\tau(x)$, the diffusivity D_p and therefore the coefficients $P_\pm(x)$.

Moreover, the Monte Carlo approach allows to define all the relevant simulation parameters involving both the experimental setup, such as the lateral or frontal irradiation geometry, the number N_P of ions per generation position, the number N of EHPs per simulated ion, and the induced charge pulse detection and processing, such as the lateral beam dispersion, the electronic noise and threshold [10]. Additionally, the ionization profile required as input for the simulation of frontal IBIC experiments can be imported from dedicated simulation software [13].

The stochastic approach allows the IST to simulate each ion hit as an independent event, and to evaluate statistical mean and median profiles of the CCE distribution. Furthermore, due to the time-dependence of the continuity eq. (2), the time-resolved CCE rise is calculated without any additional computational cost.

CCE degradation in irradiated devices

The IST includes a recently developed model [6] describing the radiation effects on the electronic properties in silicon devices. The model relates the carrier lifetime profile $\tau(x)$, and therefore the CCE degradation in the device, to the volume vacancy density $V(x)$ induced by ion irradiation:

$$\frac{\tau_0}{\tau(x)} = 1 + \tau_0 \cdot V(x) \cdot k \cdot \sigma \cdot v_{th} \tag{4}$$

where τ_0 is the lifetime in the pristine material, σ is the carrier trapping cross section, v_{th} is the thermal velocity and k is number of electrically active traps generated per radiation-induced vacancy. Therefore, k can be regarded as the quantitative parameter defining the radiation hardness of a material. The vacancy density profile $V(x)$ can be obtained multiplying the vacancy density profile per damaging ion $W(x)$ by the ion fluence Φ, $V(x) = W(x) \cdot \Phi$. The evaluation of $W(x)$ can be performed by ad hoc Monte Carlo codes such as SRIM [13]. The model provides a description of the carrier lifetime degradation in low irradiation conditions, i.e. assuming a linear dependence on ion fluence, and it does not take into account for irradiation-induced modifications of the electrostatics of the device. As the model in eq. (4) can be naturally implemented in the IST through the expression for $P_\tau(x)$ in eq. (3), all parameters involved are regarded as user-defined input for the simulation.

3. Experimental validation

The IST kernel has been successfully validated against preliminary benchmark experiments. In [10], the Monte Carlo simulation of a lateral IBIC experiment on a 4H-SiC Schottky diode was performed, providing an excellent quantitative agreement with the experimental median CCE median profiles, dispersion profiles and spectra.
The simulation of a frontal IBIC experiment on a multi-electrode silicon PIN detector [4] allowed to identify the contribution of the carrier species to the induced charge, proving the effectiveness of the method in a 2-dimensional geometry.

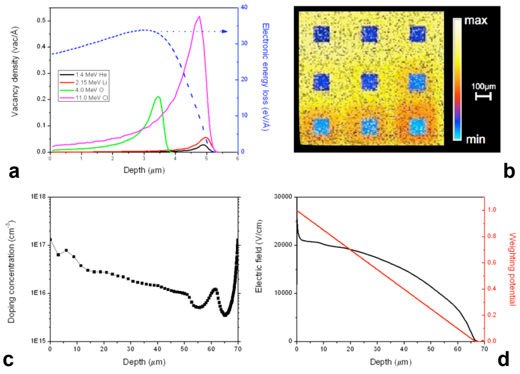

Fig. 2: **(a)** SRIM simulated vacancy production rate profiles $W(z)$ of selected ions, and electronic energy loss profile (dashed line) for 1.4 MeV He probe in silicon. **(b)** Measured 2D distribution of the IBIC signal amplitude obtained from an irradiated silicon photodiode. The nine areas irradiated at increasing ion fluence show a lower IBIC signal than the surrounding pristine material. **(c)** Doping concentration $N_D(x)$ of the pristine H-S5821 diode [6]. **(d)** Simulated electric field (black line) and weighting potential (red line) at 100 V reverse bias.

In order to test the reliability of the model for the carriers lifetime degradation presented in eq. (4), we performed a Monte Carlo analysis of a frontal IBIC experiment on irradiated silicon photodiodes. A detailed description of the experiment can be found in [6]. To summarize, nine selected areas of four identical Hamamatsu S-5821 silicon *p-n-n*$^+$ photodiodes were homogenously irradiated at different fluences in the $5 \cdot 10^7 – 5 \cdot 10^{12}$ cm^{-2} range using 1.4 MeV He, 2.15 MeV Li, 4 MeV O and 11 MeV Cl focused beams. The $W(x)$ profiles associated with each damaging ion specie are shown in Fig. 2a. The irradiated areas were investigated by IBIC microscopy (Fig. 2b) using a 1.4 MeV low current (<fA) He microbeam in fully depletion configuration (reverse bias of 100 V). The ionization profile associated with the ion probe is shown in Fig. 2a. The fitted average value of measured IBIC spectra extracted from the central part of irradiated areas (blue shadded squares in Fig. 2.2), was normalized to the mean IBIC value in the pristine material in order to obtain the relative CCE degradation for that particular accumulated dose. The obtained CCE(Φ) distributions shown in Fig. 3 (black triangles) exhibit a decrease of the CCE at increasing irradiation fluences.
A Monte Carlo simulation of the experiment was performed using the 1.4 MeV He ionization profile in silicon shown in Fig. 2a. The doping concentration profile extracted from capacitance-voltage measurements (Fig. 2c) was exploited to define the input electrostatic model of the device (Fig. 2d) using an external finite element method solver; coefficients $P_\pm(x)$ were evaluated assuming typical values of mobility (μ_n=1350 cm^2/V/s, μ_p=450 cm^2/V/s) and saturation velocity (~10^7 cm/s for both carriers), where to following expression for the high field mobility was adopted:

$$\frac{\mu}{\mu_0}=\sqrt{1+\left(\frac{\mu_0 E(x)}{v_{sat}}\right)^2} \qquad (5)$$

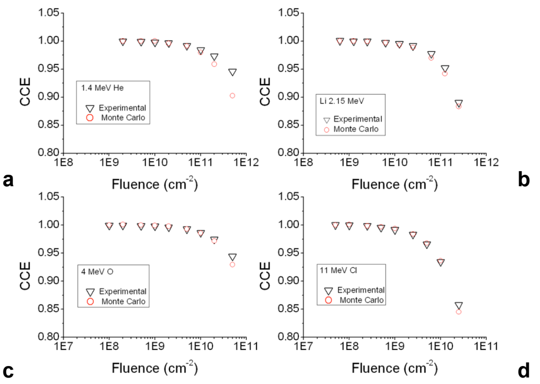

Fig. 3: Experimental (black triangles) and Monte Carlo (red circles) median CCE values measured in 1.4 MeV He IBIC experiments on four H-S5821 diodes irradiated at increasing fluences by **(a)** 1.4 MeV He, **(b)** 2.15 MeV Li, **(c)** 4 MeV O, **(d)** 11 MeV Cl. Monte Carlo were values simulated assuming k=0.18.

The lifetime profiles in the damaged diodes were calculated at each value of Φ through eq. (4), where $W(x)$ was extracted from the SRIM simulations in Fig. 2a, and τ_0, σ v_{th} were set to 10 µs, $5\cdot10^{-15}$ cm^2 and 10^7 cm/s for both carriers, respectively.

The Monte Carlo simulation was performed setting N=1000 EPHs, and considering N_p=500 independent ions at each irradiation fluence. No beam dispersion and electronic noise and threshold were considered.

The simulated mean CCE values (red circles) are compared with the experimental data (black triangles) in Fig. 3. The experimental findings for all four studied probe-damage cases were satisfactorily reproduced assuming k=0.18. The same value for the parameter k, i.e. the number of electrically active traps generated per radiation-induced vacancy, was obtained in [6] using the Shockley-Ramo-Gunn formalism [8], without statistical Monte Carlo approach. The results of the simulation reinforce the proposed interpretational model and validate the effectiveness of its Monte Carlo implementation.

4. Discussion

In this paper we reported on the progress in the development of a GUI-equipped Monte Carlo software [12] for the simulation of IBIC experiments, offering the full control of the main transport, simulation and irradiation parameters.

The IST implements a recently proposed model [6] for the interpretation of low-fluence radiation damage effects on the carriers' lifetime in semiconductors and insulators.

The model was successfully tested against a benchmark IBIC experiment on silicon photodiodes irradiated at increasing fluences by different ion species. The IST reproduced the experimental findings, assuming electrostatic, charge transport and radiation hardness properties comparable to those in [6], thus confirming the effectiveness of the model implementation.

The versatility of the stochastic approach allows a straightforward extension to higher dimensional geometries, and the adoption of additional refined models for trapping kinematics, Finally, the effectiveness of the IST implementation provides a resource for IBIC experiments simulation and offers an interpretational support to evaluate the radiation hardness of materials and devices.

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