STATISTICAL ANALYSIS FOR THE THREE-DIMENSIONAL MONTE CARLO SIMULATION OF ION IMPLANTATION

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ABSTRACT

Without a proper statistical analysis of the simulation output data, it is not possible to assess the statistical accuracy of three-dimensional Monte Carlo simulation results. The Monte Carlo technique applied to the simulation of ion implantation produces a statistical fluctuation of the doping profile, in particular in the three-dimensional case. The statistical accuracy is determined basically by the number N of simulated ion trajectories. It depends also on the variation of the ion concentration up to several orders of magnitudes in the simulation domain. The theoretical simulation error of order $1/\sqrt{N}$ has been expectedly verified by several simulation experiments with different N. The paper describes the application of statistical methods in order to evaluate the accuracy of three-dimensional ion implantation results compared to one-dimensional results. We propose a method to determine the number of trajectories required to obtain a specified precision in a three-dimensional Monte Carlo simulation study.

INTRODUCTION

Ion implantation is the state-of-the-art method for doping semiconductors because of its high controllability. The small dimensions of modern semiconductor devices have led to simulation applications which require a high accurate and full three-dimensional treatment. Since the process of ion implantation has a statistical nature, it is straightforward to use statistical methods to simulate it on computers. The most important of such methods is the Monte Carlo method which is based on applying random behavior at an atomistic level (Hobler and Selberherr 1989), (Ziegler et al. 1995).
Particularly, the position where an ion hits the crystalline target is calculated using random numbers. Furthermore, the lattice atoms of the target are in permanent movement due to thermal vibrations. Thus, the actual positions of the vibrating atoms in the target are also simulated using random numbers. The trajectory of each implanted ion is determined by the interactions with the atoms and the electrons of the target material. The final position of an implanted ion is reached where it has lost its complete energy. The accuracy of the simulation is mainly determined by the complexity of the models that describe the physical behavior. These models are applicable for a wide range of implantation conditions without additional calibration. The number of simulated ions must be considerably increased in order to achieve the same statistical accuracy for three-dimensional simulations as in two dimensions. Therefore the computational effort grows approximately proportional to the surface area of the simulation domain. A very common mode of operation is to simulate an arbitrary large number N of ion trajectories and then treat the resulting ion concentration estimates as the exact doping profile. In spite of the use of an expensive simulation model misleading results might be obtained, if the random nature of the output data is ignored. From our point of view no in-depth analysis of the simulation accuracy of Monte Carlo process simulations has been carried out so far, and in this work we will present the first comprehensive investigation of the statistical accuracy for three-dimensional Monte Carlo simulations of ion implantation.

The practitioner of a Monte Carlo simulation is always concerned with the computational time and the statistical accuracy of the simulation. Both are related to the simulation rate of convergence to the "true" value. The standard error in the simulation can be viewed as the standard deviation of the random sample divided by an increasing function of N, the number of simulated ions. We assume that all simulated ions are statistically independent. One way to reduce the simulation error is by using a smart postprocessing of the row data. The statistical fluctuation can be reduced effectively by smoothing the Monte Carlo simulation results in a postprocessing step (Heitzinger et al. 2003). The other obvious way to reduce the error is by increasing the number N of simulated ions. The traditional Monte Carlo technique using pseudo random numbers has only a convergence rate of order $1/\sqrt{N}$, which follows from the Central Limit

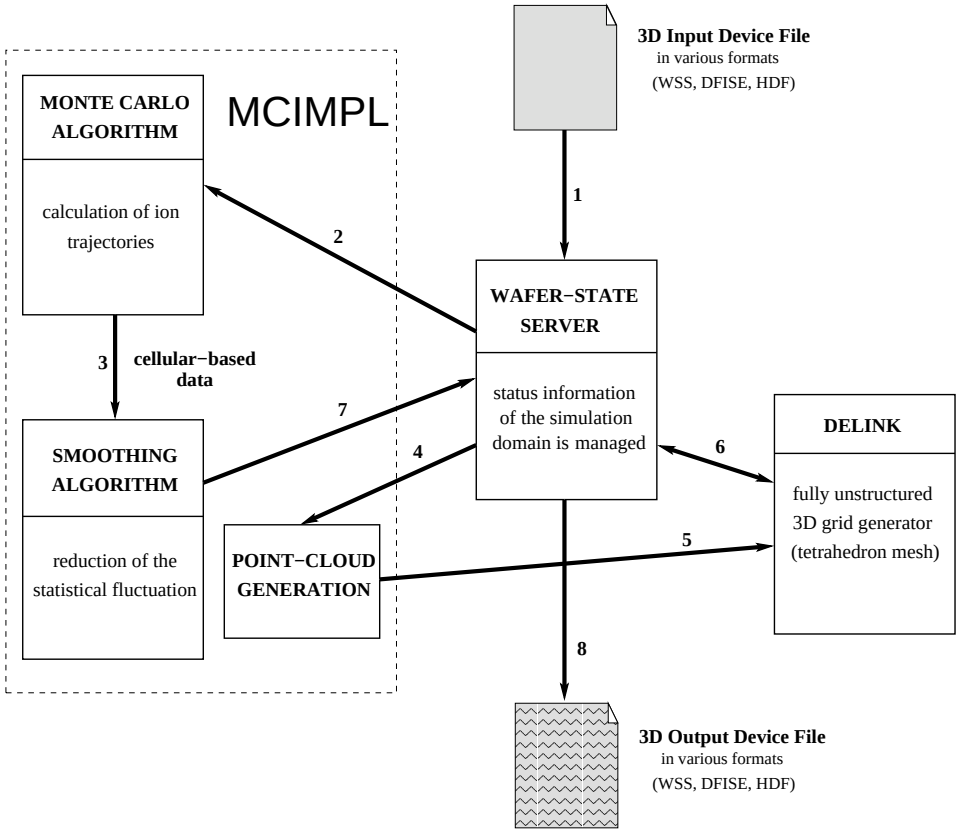

Figure 1: Data flow and involved process simulation tools.

Theorem (Law and Kelton 2000). This rate is independent of the dimension and depends only on the number N of simulations.
However, there is always a trade-off between the computational effort and the simulation error. In particular with regard to three-dimensional Monte Carlo simulations additional speed-up techniques have to be used in order to get reasonably low statistical noise by practicable long simulation runs. Examples of such speed-up techniques are the trajectory split method and the trajectory reuse method.

THE SIMULATOR

All Monte Carlo simulation experiments were performed with the object-oriented, multi-dimensional ion implantation simulator MCIMPL. The simulator is based on a binary collision algorithm and can handle arbitrary three-dimensional device structures consisting of several amorphous materials and crystalline silicon. In order to optimize the performance, the simulator uses cells arranged on an ortho-grid to count the number of implanted ions and of generated point defects. The final concentration values are smoothed and translated from the internal ortho-grid to an unstructured grid suitable for subsequent process simulation steps, like finite element simulations for annealing processes.
Figure 1 shows the data flow during the simulation of ion implantation. The simulator MCIMPL is embedded in a process simulation environment by using the object-oriented WAFER-STATE SERVER library (Binder and Selberherr 2003).
The WAFER-STATE SERVER has been developed in order to integrate several three-dimensional process simulation tools used for topography, ion implantation, and annealing simulations. It holds the complete information describing the simulation domain in a volume mesh discretized format, and it provides convenient methods to access these data. The idea was that simulators make use of these access methods to initialize their internal data structure, and that the simulators report their modifications of the wafer structure to the WAFER-STATE SERVER. Thereby a consistent status of the wafer structure can be sustained during the whole process flow.
The meshing strategy of DELINK follows the concept of advancing front Delaunay methods and produces tetrahedral grid elements (Fleischmann and Selberherr 2002).

ANALYSIS METHOD

For the analysis of three-dimensional simulation output, several numerical experiments were performed on a three-dimensional structure equivalent to a one-dimensional problem. In particular, implantations of phosphorus ions into a crystalline silicon substrate were

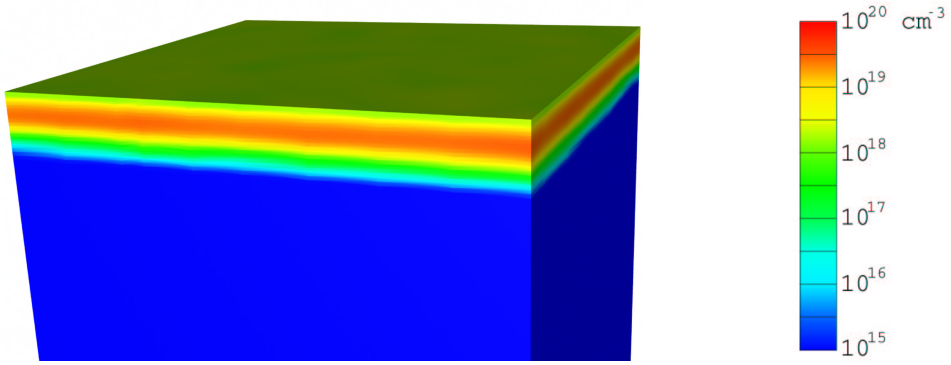

Figure 2: Accurate Monte Carlo simulation result of phosphorus implantation in silicon with $N = 10^7$ simulated ions, an energy of 25 keV, and a dose of 10^{14} cm^{-2}.

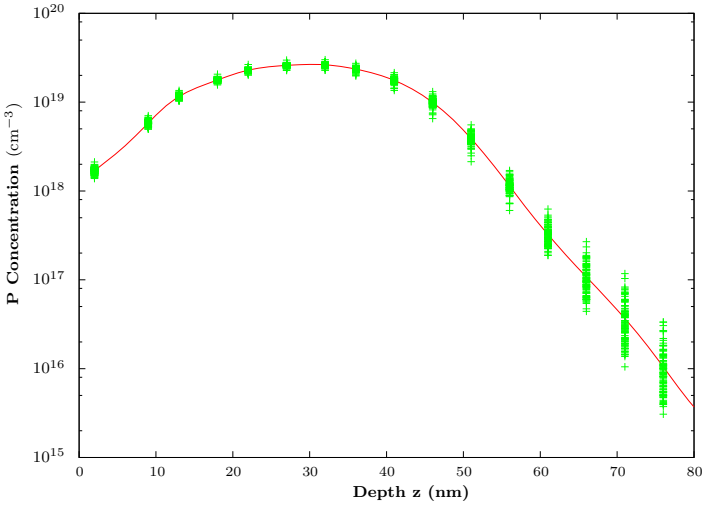

Figure 3: Variability of the three-dimensional result.

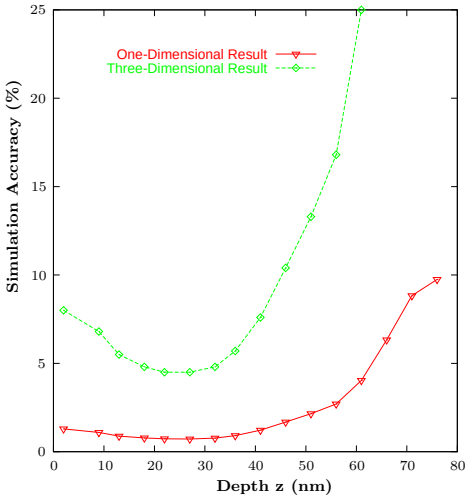

Figure 4: Result evaluation.

simulated with different N. Figure 2 shows the three-dimensional result for an accurate simulation with $N = 10^7$ ions. We extracted the z coordinates and the phosphorus concentration values C (vertical direction) from all 2972 grid points of the unstructured grid. This leads to Figure 3 which demonstrates the statistical fluctuation of the impurity concentration at equal penetration depth z.

The relative standard deviation of the impurity concentration in a plane $z = \text{const}$ is a measure for the simulation error of three-dimensional results compared to one-dimensional results. The mean impurity concentration $\overline{C}(n)$ of n grid points at equal location z forms the one-dimensional doping profile. The standard deviation $S(n)$ of a sample defined by the concentration values of n grid points in a plane $z = \text{const}$ is given by

$$S(n) = \sqrt{\frac{\sum_{i=1}^{n}[C_i - \overline{C}(n)]^2}{n-1}} \tag{1}$$

$$\sigma = \frac{S(n)}{\overline{C}(n)} \tag{2}$$

The relative standard deviation σ according to (2) is calculated in order to evaluate the three-dimensional result.

Figure 4 demonstrates the statistical accuracy of the three-dimensional result related to the one-dimesional doping profile. Most of the simulated ions come to rest close to the mean projected range R_p, causing a small variance there. Due to the very low dopant concentration in deeper regions (typically more than 10^4 times lower than at the maximum), insufficient events lead to an increase of the statistical noise.

Being based on random numbers, the results obtained with the Monte Carlo technique are never exact, but rigorous in a statistical sense. The results converge to the used model characteristics. A 90% confidence interval is constructed for the mean, in order to assess the relative error of the one-dimensional doping profile in relation to the model limit value. The half of the approximate 90% confidence interval, $\Delta(n)$, using the t distribution (Law and Kelton 2000) is given to

$$\Delta(n) = t_{n-1,0.95}\,\frac{S(n)}{\sqrt{n}} \tag{3}$$

The relative statistical error $\epsilon(n)$ for the one-dimensional doping profile can be defined as

$$\epsilon(n) = \frac{\Delta(n)}{\overline{C}(n)} \tag{4}$$

The assessed statistical accuracy of the one-dimensional doping profile according to (4) is also demonstrated in Figure 4.
The accuracy of the Monte Carlo result is determined by the number of counted ions per cell. The distribution of N ions determines the one-dimensional doping profile by using a scaling factor α:

$$\alpha \int_0^\infty \overline{C}(z)dz = N \tag{5}$$

(5) can be used in order to calculate the factor α by means of numerical integration. For a small volume of the width Δz (cell dimension) the local number N_i of simulated ions is determined by

$$N = \sum_i N_i, \qquad N_i = \alpha\, \overline{C}_i\, \Delta z \tag{6}$$

The division by all cells of a z plane yields to the average ions per cell, which is demonstrated in Figure 5 for N = 10^7 simulated ions. Each bar is located at the grid points of the internal ortho-grid. The histogram demonstrates that in deep regions only one simulated ion per cell is available in the mean. More and more empty cells at increasing penetration depth downgrade the statistics dramatically.

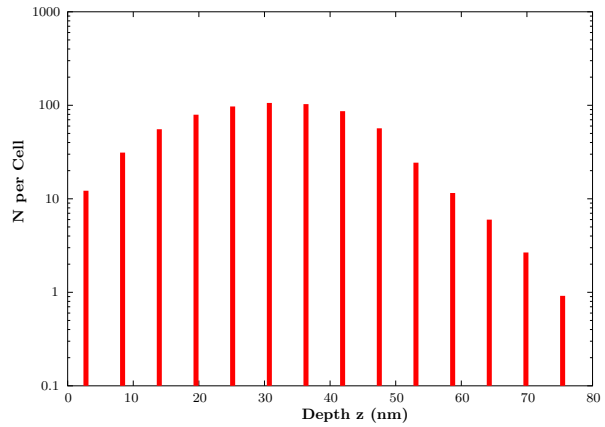

Figure 5: Estimated simulated ions per cell for a total number N = 10^7.

An essential contribution to the accomplished accuracy of the final result is obtained through the reduction of the statistical fluctuation by an implemented smoothing algorithm (Heitzinger et al. 2003). This algorithm sweeps a small rectangular grid over the points of the new tetrahedral grid and uses an approximation by generalized Bernstein polynomials. The Bernstein approximation of a concentration value on a new grid point by using the values of cells located close to the new grid point reduces significantly the statistical noise. The bad statistics generated by empty cells can be attenuated by averaging the values of surrounding cells.
We extracted again z coordinates and phosphorus concentration values from all $120 \times 112 \times 20$ cells of the simulation area. Figure 6 compares the relative standard

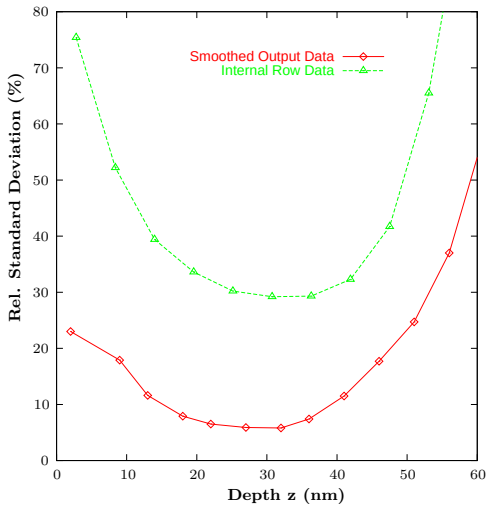

Figure 6: Improvement of the statistical accuracy by smoothing ($N = 10^6$).

deviation for $N = 10^6$ ions before and after smoothing. Thus a significant improvement of the statistical accuracy of Monte Carlo results can be achieved through the filter effect of the Bernstein polynomials, which eliminates high-frequency fluctuations from the original data.

Of great importance for the simulation is the weight of an ion, which is defined by the ratio of the number of real ions N_{real} to the number of simulated ions N.

$$Weight = \frac{N_{\text{real}}}{N} \tag{7}$$

In our simulation experiment shown in Figure 2 the surface dimension is 0.7μm x 0.65μm. With a dose of 10^{14} cm^{-2}, 455000 ions are implanted. With 10^7 simulated ions the weight of an ion results to 0.0455. In practice the real-world implanted doping profile has also a fluctuation due to the statistical nature of the implantation process. In our simulation example a real ion has only a very little weight. Thus the simulation result can be considered as a simulation of averaging over multiple real-world implantations.

IMPROVEMENT OF THE SIMULATOR

The crucial factor for the duration and accuracy of the simulation is the specified number N of ion trajectories as input data of the simulator. One drawback of the fixed-sample-size procedure based on N simulated ions is that the analyst has no immediate control over the precision of the output data. We suggest an improvement of the used fixed-sample-size procedure by determining the duration of the simulation also through a specified precision as input data of the simulator.
The simulation error of the Monte Carlo method is of order $1/\sqrt{N}$. The relationship between the standard deviation σ and the number N of ions is given by

$$\sigma = const \cdot \frac{1}{\sqrt{N}} \tag{8}$$

This relationship has been expectedly verified by simulation experiments with different N and is demonstrated in Figure 7. It can also be used to assess the number of trajectories required to obtain a specific precision in a Monte Carlo simulation study.

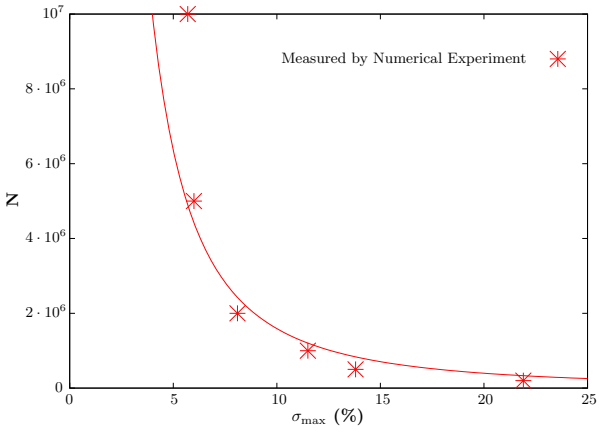

Figure 7: Required N as a function of the desired three-dimensional accuracy .

As measure of the simulation accuracy, the desired maximum of the relative standard deviation $\sigma_{\max}$ within the range $2{\cdot}\Delta R_{\mathrm{p}}$ (twice the straggling at the mean projected range) of the doping profile is used. In our experiment of Figure 2, $2 \cdot \Delta R_{\mathrm{p}} = 22$ nm at $R_{\mathrm{p}} = 30$ nm.
For the calculation of the required N as function of the given standard deviation $\sigma_{\max}$, a parameter γ is used which takes the incident atom species and the implantation energy into account. The following formula can be used to assess the N for a specified surface area A and a desired precision $\sigma_{\max}$:

$$N = \gamma \, \frac{\mathrm{A}}{\mathrm{A}_0} \, \frac{1}{\sigma_{\max}^2}, \qquad A_0 = 0.455 \ \mu\mathrm{m}^2 \tag{9}$$

Figure 7 demonstrates this relationship for a phosphorus implantation, an ion energy of 25keV, $\mathrm{A} = \mathrm{A}_0$, and parameter $\gamma = 15992$.

CONCLUSION

The functionality of the three-dimensional Monte Carlo simulator MCIMPL for ion implantation is demonstrated. The statistical fluctuation of the simulation result caused by the stochastic simulation method and the expensive three-dimensional treatment are analyzed. The evaluation of the statistical accuracy for three-dimensional results is performed by the use of statistical methods like calculating the standard deviation or the confidence interval of the output data. The gained insight into the relationships responsible for the statistical accuracy is used in order to achieve a better controllability of the simulator.

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