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

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ABSTRACT

Statistical fluctuations of three-dimensional Monte Carlo simulation results require a sophisticated post-processing of the obtained data. We present an advanced algorithm for smoothing Monte Carlo results of ion implantation and translating them from the internal ortho-grid of the simulator to an unstructured grid which is suitable for subsequent process simulation steps. This algorithm allows a more accurate prediction of doping profiles, which is essential for an implantation treatment of deep-submicrometer device structures. Basically, the ion concentration value on a grid point of the unstructured grid is approximated by means of Bernstein polynomials, evaluated in a fast way only in the middle point of that cell which contains the new grid point. The key idea is to estimate also the concentration difference between the new point and the middle point by calculating the scalar product of the concentration gradient and the distance vector. In that way, effects based on the cell discretization can also be significantly reduced, which leads to more realistic doping profiles. The impact of the advanced smoothing procedure on the statistical accuracy for three-dimensional implantation applications is demonstrated.

INTRODUCTION

Ion implantation is the most important doping technique for electronic device fabrication, in particular for ultra large scale integration (ULSI) circuits. The ongoing trend of scaling device feature sizes down to the deep-submicrometer regime requires TCAD tools which provide a more accurate prediction of doping profiles and a full three-dimensional implantation treatment.

These requirements drive the improvement and optimization of existing three-dimensional Monte Carlo simulation tools in the field of ion implantation.

The Monte Carlo method 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. In this model the ion implantation process is accurately simulated by computing a large number N of individual ion trajectories through a semiconductor material. The trajectory of each implanted ion is determined by the interactions with the atoms and electrons of the target material. The final position of an implanted ion is reached where it has lost its kinetic energy. The crystalline model of silicon allows to simulate the channeling effect during ion implantation. Additionally, point defect distributions generated as results of ion implantation can also be calculated by the Monte Carlo approach. The Monte Carlo method to model ion implantation has the advantage of being a physically based method and therefore it is easily extendable for new technological conditions without the need for additional extensive calibration. On the other hand, long computing times prevent the standard use of Monte Carlo simulation tools in technology optimization.

Based on random numbers, the results obtained with the Monte Carlo method are never exact but rigorous in a statistical sense. The results converge to the used model characteristics by increasing the number N of simulated ions. As with experiments, the errors on Monte Carlo results are divided into two classes: statistical errors and systematic errors.

The statistical error is basically determined by the number N of calculated trajectories. The slow convergence rate of the Monte Carlo method leads to long simulation runs and produces ion concentration
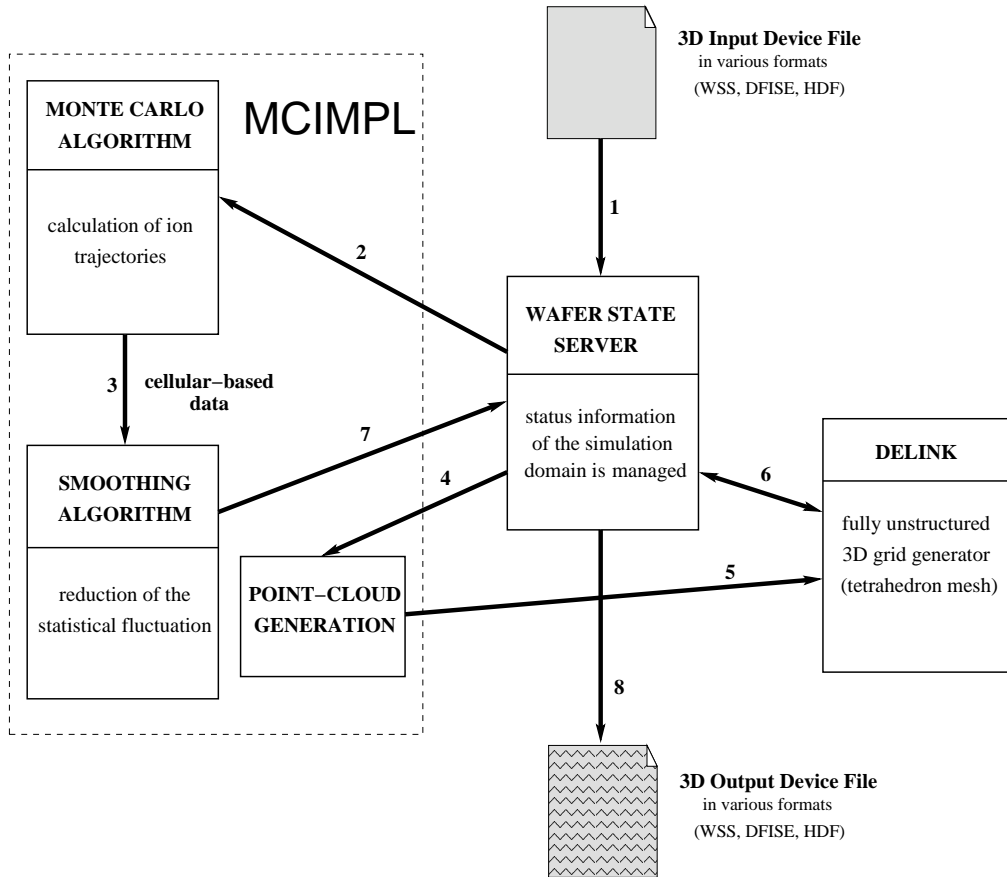
Figure 1: Data Flow and Involved Process Simulation Tools

estimates which tend to have high variances. The obvious way to reduce the statistical error is by increasing the number N of simulated ions. This error vanishes for $N \to \infty$. Speed-up techniques like the trajectory split method (Bohmayr et al. 1995) or trajectory reuse method (Hössinger and Selberherr 1999) help to increase N by holding the additional computational effort within acceptable limits.

On the other hand, systematic errors arise due to model limitations or insufficient calibration of the simulator. Model validation or software verification will not be covered in this work.

Paticularly in three-dimensional applications a worse statistical representation arises in regions with a dopant concentration several orders of magnitudes smaller than the maximum (projected range). The raw Monte Carlo results are smoothed through a post-processing step in order to achieve results with an acceptable accuracy even in deep regions with a poor statistical representation of dopants. It turned out that fluctuations of the original data can effectively be reduced by using an approximation with Bernstein polynomials. We have developed an advanced smoothing algorithm which extends the Bernstein approximation by calculating an additional linear approximation also in a fast manner. This algorithm

helps to significantly reduce the statistical error of three-dimensional Monte Carlo simulation results.

THE SIMULATOR

All Monte Carlo simulation experiments were performed with the object-oriented, multi-dimensional ion implantation simulator MCIMPL-II. 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-II is embedded in a process simulation environment by using the object-oriented WAFER STATE SERVER library (Binder and Selberherr 2003), (Binder et al. 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 is that simulators make use of these access methods to initialize their internal data structures, 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).

ADVANCED SMOOTHING ALGORITHM

The smoothing of the raw Monte Carlo result is performed by approximating the concentration value on a grid point of the unstructured grid by means of Bernstein polynomials defined in a cubical surrounding space (Heitzinger et al. 2003). The Bernstein polynomial $B_{f,n,n,n}(x_1, x_2, x_3)$ approximates a function f of 3 variables, where $n \in \mathbf{N}$ are the concentration sample points in each dimension. The Bernstein approximation $B_{f,n,n,n}$ is specified by n^3 sample points whereby $B_{f,n,n,n}$ does not run through the sample points, but each of them affects the approximated function. Such sample points are usually called control points, since they enforce the function progression.

The statistical accuracy of the Monte Carlo result is determined by the number of counted ions per cell. More and more empty cells at increasing penetration depth downgrade the statistics dramatically. The calculation of the Bernstein approximation needs a reasonable information in all sample points. In order to fulfill this requirement, the concentration value at a sample point in an empty cell is calculated by averaging over the values of surrounding cells.

It is not necessary to calculate the Bernstein polynomial explicitly, since each polynomial is only evaluated in the middle point $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ of the domain $[0, 1]^3$. In this case, the approximating polynomial of order $(n^3 - 1)$ can be simplified to the formula according to (1), which enables a fast calculation of the approximated value.

$$B_{f,n,n,n}\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) =$$
$$= \sum_{k_1=0}^{n} \sum_{k_2=0}^{n} \sum_{k_3=0}^{n} f_{k_1,k_2,k_3} \binom{n}{k_1}\binom{n}{k_2}\binom{n}{k_3} \left(\frac{1}{2}\right)^{3n} \quad (1)$$

For the original smoothing algorithm the approximation of the concentration values for the grid points of
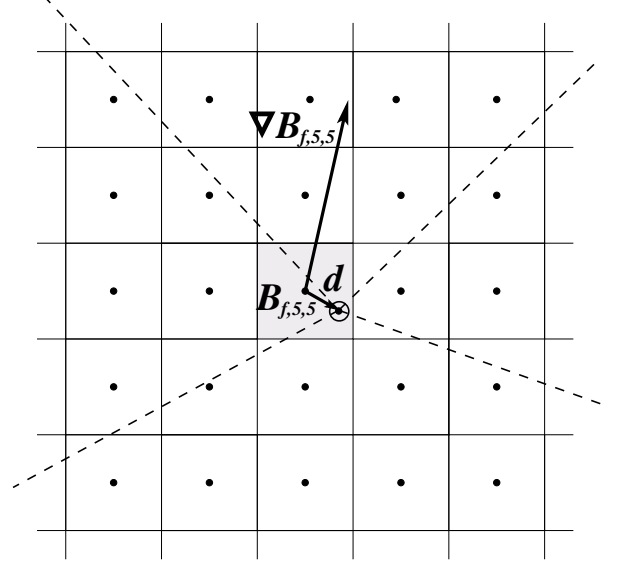

Figure 2: This sketch demonstrates the calculations performed for one point of the new unstructured grid in a two-dimensional example. It can be applied to the third dimension in an analogous manner. The thin orthogonal lines confine the cells of the internal grid. The four dashed lines denote the unstructured grid, where the new point is marked by a small circle. In the first step the 5^2 sample points are used to calculate the concentration value $B_{f,5,5}$ at the middle of the central grey cell. Then the scalar product of the gradient and the distance vector $\mathbf{d}$ is calculated to produce a delta concentration value.

the unstructured grid was evaluated only in the middle point of that cell which contains the grid point. The drawback is that two grid points contained in the same cell get an equal concentration value. This approximation can be improved if the distance of the new point from the middle point is also taken into consideration as it is depicted in Figure 2. According to (2) the concentration difference $\Delta B_{f,n,n,n}$ between the new point and the middle point can be approximated by the scalar product of the concentration gradient and the distance vector. (3) points out that it is possible to calculate the required three partial derivatives also in a fast way.

$$\Delta B_{f,n,n,n} = \nabla B_{f,n,n,n} \cdot \mathbf{d} \quad (2)$$

$$\left.\frac{\partial}{\partial x_i} B_{f,n,n,n}\right|_{\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)} =$$
$$= \sum_{k_1=0}^{n} \sum_{k_2=0}^{n} \sum_{k_3=0}^{n} f_{k_1,k_2,k_3} \binom{n}{k_1}\binom{n}{k_2}\binom{n}{k_3} \cdot$$
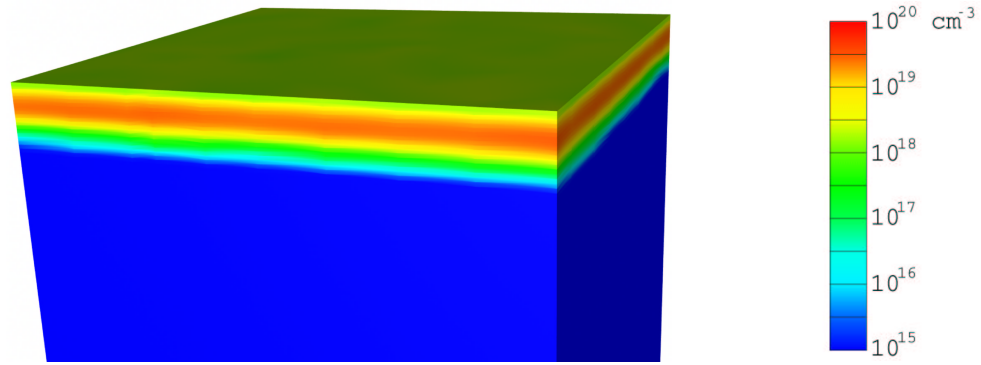$$\cdot \left(\frac{1}{2}\right)^{3n} (4k_i - 2n) \quad (3)$$

Figure 3: Accurate Monte Carlo Simulation Result of Phosphorus Implantation in Silicon with $N = 4 \cdot 10^6$ Simulated Ions, an Energy of 25 keV, and a Dose of 10^{14} cm^{-2}
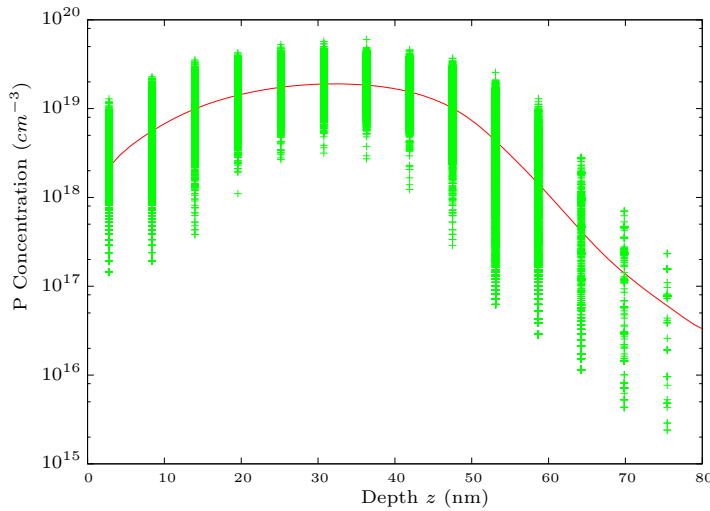

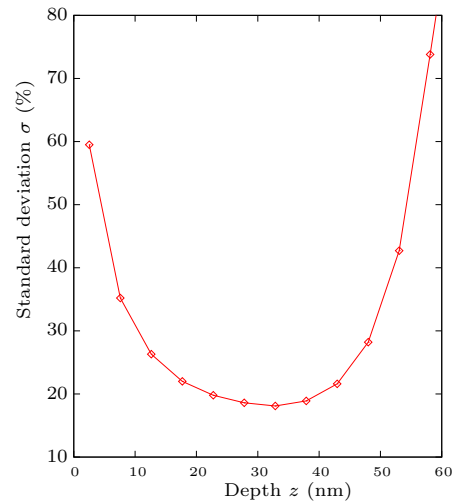Figure 4: Fluctuation of the Raw Monte Carlo Result
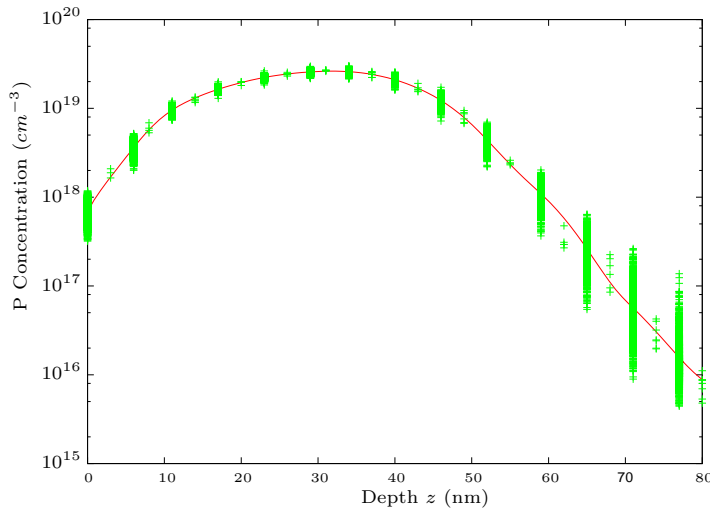

Figure 5: Raw Result

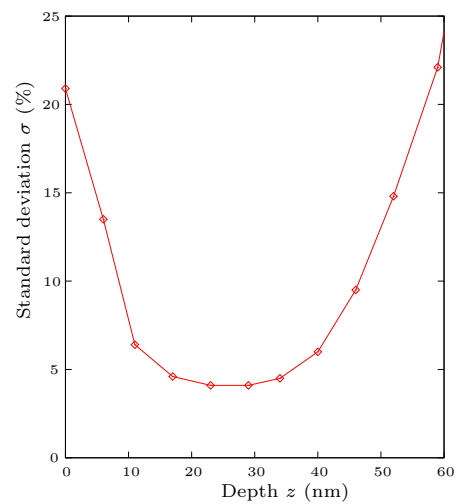Figure 6: Fluctuation of the Smoothed Simulation Result

Figure 7: Smoothed Result

For the analysis of the implemented smoothing algorithm, numerical experiments were performed with the simulator MCIMPL-II on a three-dimensional structure equivalent to one-dimensional problems. We assume that all simulated ions are statistically inde-

pendent. Figure 3 shows the three-dimensional result for the implantation of phosphorus ions into a crystalline silicon substrate with $N = 4 \cdot 10^6$ simulated ions. We extracted z coordinates and phosphorus concentration values C (vertical direction) from

all $120 \times 112 \times 20$ cells of the simulation area. This leads to Figure 4 which shows a significant statistical fluctuation of the ion concentration at equal penetration depth z for $N = 4 \cdot 10^6$ ions. The relative standard deviation σ 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 (Figure 5). The mean impurity concentration $\overline{C}(n)$ of n ortho-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

$$S(n) = \sqrt{\frac{\sum_{i=1}^{n}[C_i - \overline{C}(n)]^2}{n-1}} \qquad (4)$$

$$\sigma = \frac{S(n)}{\overline{C}(n)} \qquad (5)$$

The relative standard deviation σ according to (5) is calculated in order to evaluate the three-dimensional raw Monte Carlo result before smoothing. Additionally, we extracted all z coordinates and smoothed phosphorus concentration values from the unstructured grid. This leads to Figure 6 which shows a clearly reduced fluctuation of the phosphorus concentration compared to Figure 4. Most of the ions come close to the mean projected range R_p to rest, causing a smaller variance there. Figure 7 shows the corresponding relative standard deviation σ of the final simulation result.

As measure of the improvement, the ratio of the maximum of the 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, after and before smoothing, can be used. In our case $\sigma_{\max,\text{after}}/\sigma_{\max,\text{before}} = 0.25$ for $2 \cdot \Delta R_\mathrm{p} = 22$ nm at $R_\mathrm{p} = 30$ nm.

$$\sigma_{\max} = const \cdot \frac{1}{\sqrt{N}} \qquad (6)$$

The theoretical simulation error $\sigma_{\max}$ according to (6) follows from the Central Limit Theorem (Law and Kelton 2000). It has been expectedly verified by simulation experiments with different N (Wittmann et al. 2003). In order to reduce $\sigma_{\max}$ by $1/4$ only by increasing N, one has to increase N by a factor of 16. But as demonstrated in Figure 4–7 also a significant improvement of the statistical accuracy can be achieved by sophisticated postprocessing, in particular through the filtering effect of the Bernstein polynomials, which eliminates high-frequency fluctuations from the original data.

The linear approximation of the delta concentration value between the grid point of the unstructured grid
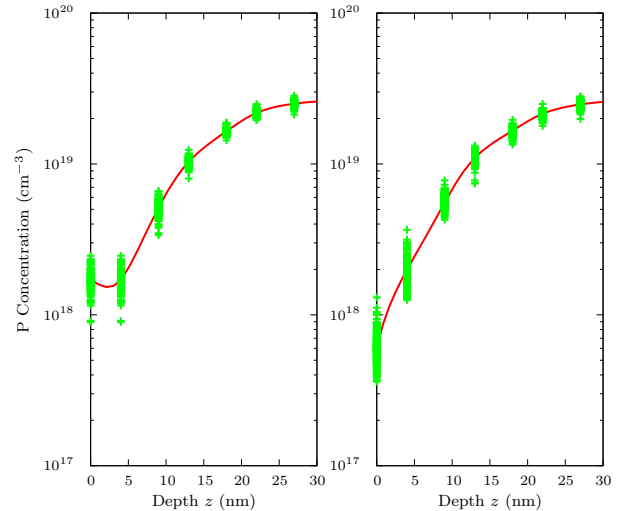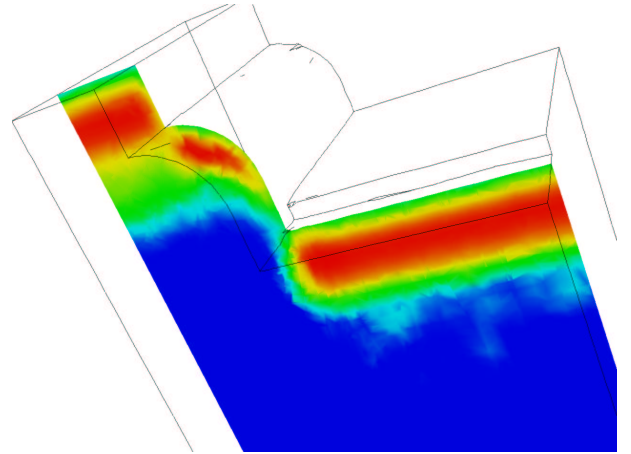

Figure 8: Effect of the Linear Approximation

Figure 9: Monte Carlo Implantation Application

and the associated cell middle point significantly reduces the effect of the cell discretization. A rough cell dimension (5 nm) is used for the Monte Carlo simulation to count the number of implanted ions in a computationally efficient way. The left part of Figure 8 shows the doping profile produced by a Bernstein approximation without performing an additional linear approximation in the smoothing procedure. The internal cell dimension of 5 nm produces equal concentration values for the first two samples. The right part of this picture shows the doping profile obtained after advanced smoothing. As demonstrated in this comparison, the advanced smoothing algorithm leads to a smoother and therefore to a more realistic doping profile. For the year 2003 the International Technology Roadmap for Semiconductors (Semiconductor Industry Association 2001) predicted the necessity of a simulation accuracy of 5% (5 nm) for vertical and lateral junction depths. Longer computing times or worse statistics would arise if the cell dimension of the simulator would be further reduced under 5 nm

in order to enhance the accuracy. In contrast to that the used smoothing algorithm can help to improve the accuracy of Monte Carlo results in a computationally efficient way.

Figure 9 shows the result of an implantation performed with the simulator MCIMPL-II. In this application a real-world device stucture for processing a MOS transistor was used as input of the simulation. Arsenic ions with an energy of 70 keV and a dose of $3 \cdot 10^{15}$ cm^{-2} were implanted. In this example only 2000000 initial ions were used to demonstrate the fluctuation of the doping profile. It is recommended to use at least 2000000 ions/μm^2, otherwise the simulation result is inacceptably inaccurate due to the statistical fluctuation.

CONCLUSION

Three-dimensional Monte Carlo simulation results of ion implantation tend to inherent high variances in particular in regions with a bad statistical representation of dopants. The goal of this work is to achieve a more accurate prediction of doping profiles with the aid of advanced smoothing of Monte Carlo simulation results in a computationally efficient way. The extended algorithm has an impact on the accuracy of the predicted doping profile in various ways. High-frequency fluctuations from the original data are eliminated through the filter effect of the Bernstein polynomials in the first approximation step of the final result. Next, a linear approximation step is performed to reduce effects which arise through the cell discretization of the simulator. The analysis of the results produced by the advanced algorithm demonstrates the gained improvement of the doping profile which can immediately be used in a subsequent process simulation step.

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