A Computationally Efficient Method for Three-Dimensional Simulation of Ion Implantation

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Abstract

The high accuracy which is necessary for modern process simulation often requires the use of Monte-Carlo ion implantation simulation methods, with the disadvantage of very long simulation times especially for three-dimensional applications. In this work a new method for an accurate and CPU time efficient three-dimensional simulation of ion implantation is suggested. The approach is based on a combination of the algorithmic capabilities of fast analytical and the Monte-Carlo simulation methods.

1. Introduction

Technical requirements and user expectations for three-dimensional simulations put forward a serious challenge for the improvement of simulation methods. Three-dimensional models must be better than their counterparts in existing two-dimensional tools but at the same time a large increase of simulation time due to the three-dimensional computations and better models is not tolerable. This means that new simulation methods and better algorithms must be developed.

Traditionally there are two different approaches for the three-dimensional simulation of ion implantation. On one hand side the analytical method is established, which is based on a convolution of point response distribution functions. The three-dimensional point response distribution describes the implantation with an ideally focused ion beam. A selection of appropriate vertical and lateral distribution functions together with well calibrated parameters for a wide range of implantation conditions yield good results for many applications. Normally Gaussian, Pearson, Double Pearson functions or Pearson functions with an exponential tail are used to model the point response distribution function. Because of robust and efficient algorithms [1], the important advantage of the analytical simulation method is its short computation time, but since there is no universal set of parameters for all implantations conditions, the distribution functions have often to be re-calibrated on experimental results for the process window in question before they can be applied to specific problems.

On the other hand there is the Monte-Carlo approach which provides flexible physically based models, but the calculation time is long. When performing a Monte-Carlo

ion implantation simulation, the trajectory of each ion through the target is evaluated by calculating the interaction of the ion with the nuclei and the electrons of the target material. 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 wider range of implantation conditions without additional calibration [2], [3]. To achieve the same statistical accuracy of three-dimensional simulations as in two dimensions, the number of ions traced must be considerably increased [4]. Therefore the CPU time grows approximately proportional to the surface area of the simulation domain.

Since these two simulation methods are complementary in their capabilities, both methods have to be implemented in a professional TCAD system for micro electronic technology simulation. The main idea of this work is to integrate the analytical and the Monte-Carlo simulation methods in a manner that the advantages of both simulation methods are exploited in the most efficient way.

2. The Combined Approach

The major physical effects which have to be taken into account in an advanced simulation of ion implantation are channeling in crystalline silicon, the influence of the scattering oxide on the doping profile, and damage accumulation which results in a dose dependence of the doping profiles for heavier ions. Most of these effects are sensitive to the direction of the ion beam impact, and all of them influence each other in a non-trivial way. This complicated interaction of several effects in crystalline silicon complicates the formulation of universal analytical models while the Monte-Carlo method accounts for all these effects.

In order to comprise the larger capabilities of the Monte-Carlo method with the smaller computational requirements of the analytical method, we simulate a small but representative part of the simulation domain with the Monte-Carlo method to extract the point response function of the implanted ions. In order to correctly consider damage accumulation, a sufficiently large implantation window with a lateral size comparable to the range of the implanted ions is used for this simulation.

This numerically produced point response distribution is used instead of an analytical point response distribution in the convolution algorithm of the analytical method [5]. A reduction of the computation time compared to a full area Monte-Carlo simulation can be archived if the area of the implantation window which is used for the calculation of the Monte-Carlo point response function is small compared to the surface area of the structure for which the analytical simulation is performed. The CPU time reduction factor can be estimated as the ratio of the area filled by the point response distribution to the area of the full simulation domain and may result in a CPU time reduction by 10 to 1000. Fig. 1 shows the point response distribution for an implantation of 40 keV boron into silicon covered by 10 nm screening oxide. The point response calculated has a cudgel-like shape. The thicker part of the distribution is mainly formed by the random type scattering of the ions. The narrow strip of the distribution is formed by the channeled ions which penetrate deeper into the <110> channeling direction.

3. Simulation

A comparison of simulation results obtained by the analytical method, the combined method and the Monte-Carlo method (Fig. 2) demonstrates the increase in accuracy by using the combined method instead of a pure analytical method. We have simulated the implantation of boron ions with an energy of 40 kev and a dose of

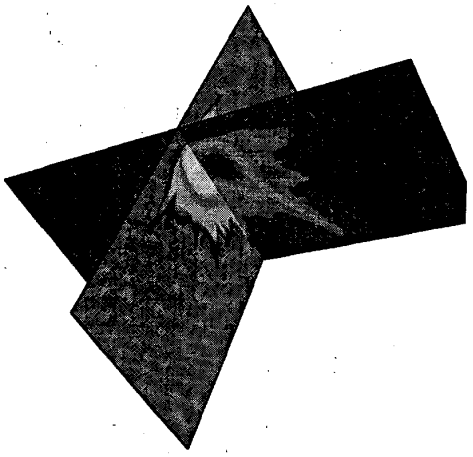

Figure 1: Two cuts through a point response function resulting from an implantation of boron ions with an energy of 40 keV and a dose of $5{\cdot}10^{13}\mathrm{cm}^{-2}$ into silicon covered with 10 nm screening oxide. The ion beam was tilted by 7° in the plane which is the lateral cut plane in the figure.

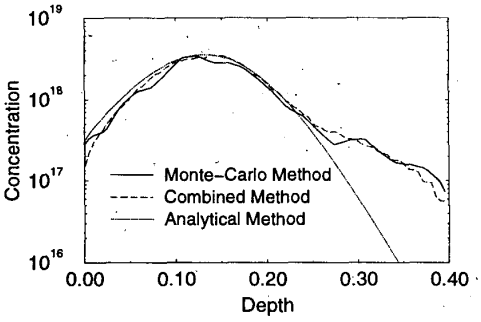

Figure 2: Simulation result of the analytical method, the combined method and the Monte-Carlo method for an implantation with boron ions with 40 keV into a one-dimensional like three-dimensional structure (a block of silicon covered by 10 nm SiO_2).

$5{\cdot}10^{13}\mathrm{cm}^{-2}$ into silicon which is partly covered by a thick silicon dioxide mask with a 45 ° tilted edge. Figure 3 shows the simulation results obtained with the analytical method using a Pearson IV point response function, with the combined approach and with a full area Monte-Carlo simulation. The size of surface of the simulation domain was 1 μm^2 while the Monte-Carlo point response function was extracted using an implantation window with a size of 0.01 μm^2. The analytical method underestimates the channeling while the doping profile calculated by the combined approach agrees very well with the Monte-Carlo simulation in the silicon region.

4. Conclusion

Using the point response function extracted from the Monte Carlo simulation we applied the CPU time effective algorithm for convolution developed earlier [5], and in this manner a point response based interface between the Monte-Carlo and analytical simulation methods was established. The simulation results of the combined approach are almost as accurate as a full area Monte-Carlo simulation but require significantly less computation time.

5. Acknowledgment

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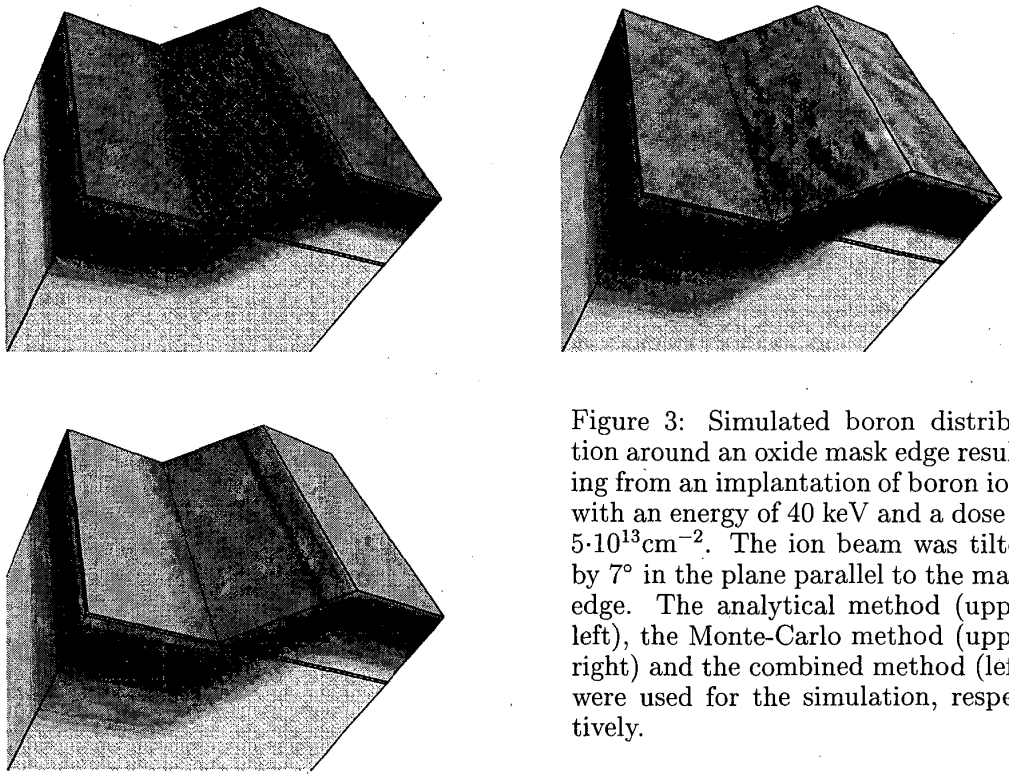

Figure 3: Simulated boron distribution around an oxide mask edge resulting from an implantation of boron ions with an energy of 40 keV and a dose of $5{\cdot}10^{13}\mathrm{cm}^{-2}$. The ion beam was tilted by 7° in the plane parallel to the mask edge. The analytical method (upper left), the Monte-Carlo method (upper right) and the combined method (left) were used for the simulation, respectively.

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