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Trajectory Split Method for Monte Carlo Simulation of Ion Implantation Demonstrated by Three-Dimensional Poly-Buffered LOCOS Field Oxide Corners

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Abstract – The benefits of an acceleration method for two and three-dimensional Monte Carlo simulation of ion implantation into crystalline targets is demonstrated by three-dimensional poly-buffered LOCOS field oxide corners. The *"trajectory split method"* ensures a much better statistical representation in regions with a dopant concentration several orders of magnitudes smaller than the maximum. As a result the time required to perform a simulation with comparable statistical accuracy is drastically reduced.

Introduction

The Monte Carlo method is rapidly gaining acceptance as a means for the simulation of ion implantation due to its capability of simulating channeling and damage accumulation phenomena in arbitrary multi-dimensional structures. A well-known disadvantage of the Monte Carlo approach is its considerable demand for computer resources to obtain results with satisfying statistical accuracy.

Recently, a "rare event" approach for one-dimensional structures [1] has been suggested to significantly improve the calculation time performance of the UT-MARLOW code [2]. Based on this algorithm our new *"trajectory split method"* delivers much better statistical accuracy in regions with a dopant concentration several orders of magnitudes smaller than the maximum (in the following we call these areas "peripheral"), it is easy to implement into existing codes, and it requires considerably less computation time to calculate implantation profiles with a given precision.

The traditional Monte Carlo approach for crystalline targets is based on the calculation of a large number of "distinct" ion trajectories, i.e. each trajectory is usually traced from the ion starting point at the surface of the target up to the stopping point of the ion. Since the majority of ion trajectories ends at the most probable penetration depth inside the structure the statistical representation of this target region is good. Peripheral areas of the dopant concentration are normally represented by a much smaller number of ions (typically 10^4 times less than at the maximum). This results in an insufficient number of events at low concentration areas and leads to statistical noise that cannot be tolerated.

The Trajectory Split Method

The fundamental ideas of our new simulation approach are to locally increase the number of calculated ion trajectories in areas with large statistical uncertainty and to utilize the information we can derive from the flight-path of the ion up to a certain depth inside the target. For each trajectory, the local dopant concentration C_{loc} is checked at certain points of the flight-path. Then we relate C_{loc} to the current maximum global concentration $C_{max,current}$ by calculating the ratio $C_{loc}/C_{max,current}$. The result is compared with given relative concentration levels (we define ten levels at 0.3, 0.09, 0.027, ..., 0.3^{10}). Only if the current local concentration falls in an interval below the previous one, a *trajectory split point* is defined at this checkpoint. Therefore our approach gives a *self-adaptive algorithm*, because more split points

are defined at areas with present unsatisfying statistical accuracy and additional trajectory branches are suppressed, when an ion moves from lower to higher local concentration levels. We store the position of the ion, its energy as well as the vector of velocity and use this data for virtual branches of ion trajectories starting at this split point. In this way the peripheral areas of the dopant concentration are represented by a much higher number of ion trajectories and the statistical noise is considerably reduced.

Implementation in VISTA

In the implementation of our method we have defined non-recursive splits of one regular ion trajectory into two virtual branches at each split point, and to obtain the correct concentration a weight was assigned to each branch. In this manner a tree of virtual trajectories is formed for each regular ion (Fig. 1).

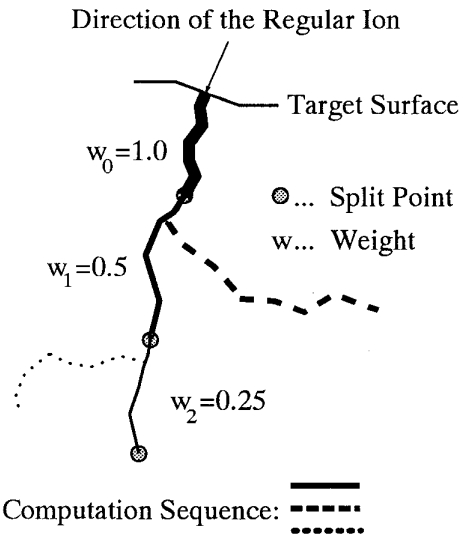

Figure 1: Topological structure of the virtual trajectory branches, their weights and their computation sequence

Such a virtual trajectory branch is calculated with the *same models and parameters* as a regular trajectory, but it starts **at the split point** with *initial conditions obtained from the regular ion.*

It should be mentioned that the different realizations of the virtual trajectories only result from the thermal vibrations of the target atoms [3].

The trajectory split approach has been implemented in the two- and three-dimensional Monte Carlo implantation modules of the VISTA framework [4]. These modules use advanced physical models [5] for calculation of ion implantation into crystalline silicon, therefore they are capable to predict the channeling effects and the transient amorphization using the modified Kinchin-Pease model [6]. To represent three-dimensional structures and to perform an efficient point-location an octree is used for geometry discretization [7] [8].

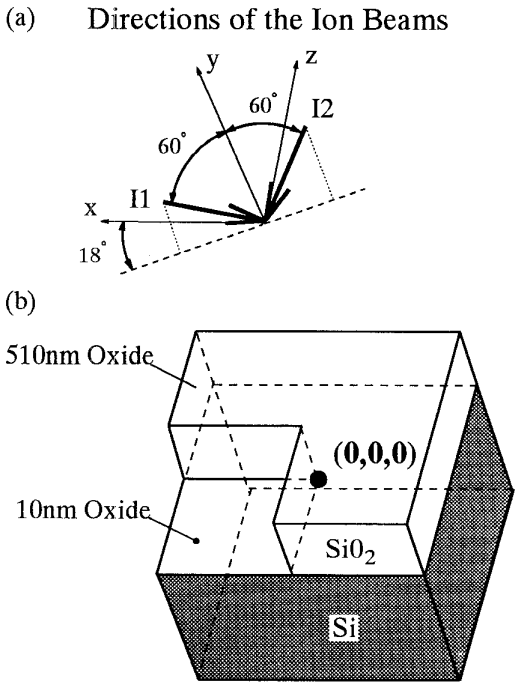

Figure 2: (a) Directions of the two ion beams (b) Poly-buffered LOCOS field oxide corner on (100) oriented single-crystal silicon

Simulation Results

To demonstrate the merits and the applicability of our new method we performed several ion implantation simulations into a three-dimensional poly-buffered LOCOS field oxide corner using the

conventional crystalline mode (Fig. 3 and Fig. 4) and the new *"trajectory split"* mode (Fig. 5 and Fig. 6). For the simulations we used a phosphorus implant of $3{\cdot}10^{13}\mathrm{cm}^{-2}$ at 50keV into (100) oriented single-crystal silicon covered by 10nm to 510nm thick oxide (see Fig. 2b). The two ion beams were tilted for 60° and −60° in the xy-plane respectively and rotated around the y-axis by 18° shown in Fig. 2a.

Comparison of the two crystalline modes with respect to the CPU time (we used a HP 735/100 workstation) needed for the *same statistical significancy* shows a clear advantage of the trajectory split method compared to the conventional one. The CPU time reduction due to the new simulation strategy is almost three times in this particular application and is inversely proportional to the statistical accuracy requirements.

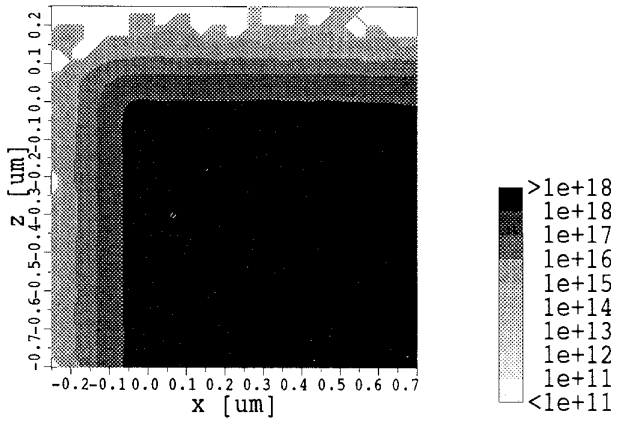

Figure 3: Concentration of Phosphorus in cm^{-3}
65nm below the silicon surface, conventional method
Ion Beam I1, CPU time: 62h 25'

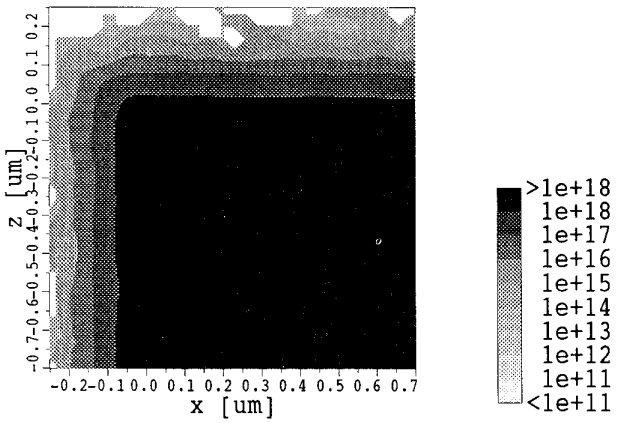

Figure 5: Concentration of Phosphorus in cm^{-3}
65nm below the silicon surface, trajectory split method
Ion Beam I1, CPU time: 23h 08'

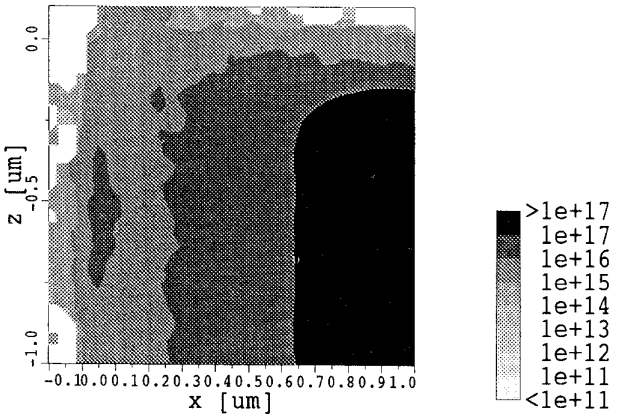

Figure 4: Concentration of Phosphorus in cm^{-3}
65nm below the silicon surface, conventional method
Ion Beam I2, CPU time: 21h 08'

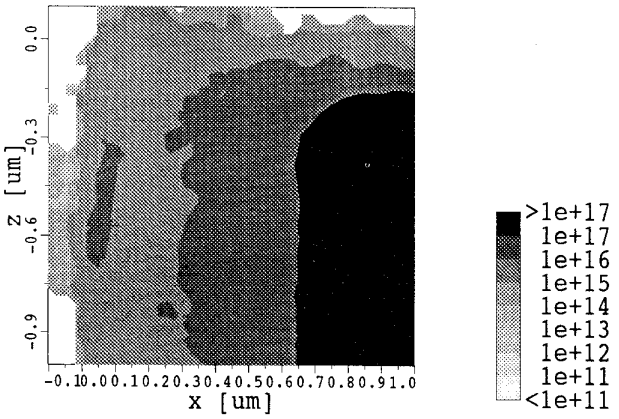

Figure 6: Concentration of Phosphorus in cm^{-3}
65nm below the silicon surface, trajectory split method
Ion Beam I2, CPU time: 7h 02'

Conclusions

We present a new acceleration method for Monte Carlo simulation of ion implantation which is applicable to arbitrary two- and three-dimensional crystalline targets. A continuous comparison between local and maximum global concentration is required by our simulation strategy. The simulation area is dynamically divided into layers each representing a certain relative concentration level of the calculated distribution. Each regular ion trajectory is traced and split into several virtual branches in case the ion leaves a concentration layer and enters another one with a lower doping.

The major advantage of the trajectory split method is a much higher statistical accuracy of the simulated ion distribution at low relative concentration. As a result, the time required to perform a simulation with comparable statistical accuracy is reduced typically by a factor of two to five in comparison to the standard approach.

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