Trajectory Split Method for Monte Carlo Simulation of Ion Implantation

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Abstract—A new method for the acceleration of two- and three-dimensional Monte Carlo simulation of ion implantation into crystalline targets is presented. 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. The advantages of the new approach have been confirmed by a thorough statistical analysis.

I. 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.

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 followed 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. Regions with a dopant concentration several orders of magnitudes smaller than the maximum (in the following we call these areas "peripheral") are normally represented by a much smaller number of ions (typically 10^4 times lower 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.

Inspired by the striking message in [1] about the results of the *rare event* approach implemented in the UT–MARLOWE code [2] for one-dimensional structures, we developed the *trajectory split method* for the Monte Carlo simulation of ion

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implantation. A similar method was first used in the work of Phillips and Price [3] to simulate hot electron transport. The algorithm drastically reduces the computational effort and is applicable for two- and three-dimensional simulations.

II. 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 ion, the local dopant concentration C_{loc} is checked at certain points of the flight-path (*checkpoints*). In order to limit the computational overhead of this strategy the checkpoints are chosen according to the following conditions: First, the ion energy has to be less than 30% of its initial value, and second, there has to be a number of ion-target collisions between two successive checkpoints. For the second parameter we use 2% of the maximum number of collisions per ion trajectory. In later versions we will replace the 30% by an energy depending threshold value to take heed of low and high energy implants. At each checkpoint 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, $\cdots$, 0.3^{10}). A *trajectory split point* is defined at this checkpoint only if the current local concentration falls in an interval below the previous one. 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.

The shape of the ion trajectory in a crystalline material is determined by two different factors: (a) The impact point of the ion into the crystal lattice, and (b) the current positions of the target atoms. The distribution of the entrance points into the silicon crystal is determined by covering layers and masks and is homogeneous for exposed crystalline surfaces. The distribution of the entrance points is determined by standard procedures [5]. The current positions of the target atoms are determined by thermal vibrations which may have a pronounced influence on the channeling and dechanneling probabilities. We have assumed a three-dimensional Gaussian distribution for the displacement of the atoms centered at the ideal sites of silicon lattice [5]. The standard deviation of the thermal vibration is 0.009 nm according to [7]. The momenta
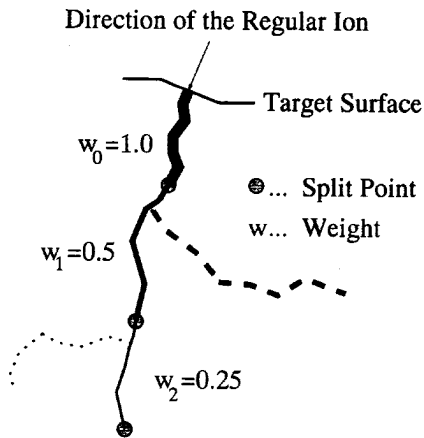
Direction of the Regular Ion

Fig. 1. Topological structure of the virtual trajectory branches and their weights.

of the lattice vibration are neglected as they are much smaller than the momentum of the ion.

In the present work, we have chosen the simplest implementation of this method by permitting only two nonrecursive virtual branches at each split point, i.e., virtual trajectories are not split once more. With this approach, the statistical behavior of the algorithm is investigated. It is expected that our method can be further improved by allowing recursive splits and by optimizing the number of virtual branches especially with respect to the given relative concentration levels and to the dimensionality of the problem. To obtain the correct concentration, a weight is assigned to each branch. In this manner, a tree of virtual trajectories is formed for each regular ion (Fig. 1). 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*. The different realizations of the virtual trajectories result from the thermal vibrations of the target atoms. 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 expected to be reduced.

As mentioned before, we subdivide the simulation area into layers each representing a certain relative concentration level. It is an important advantage of the trajectory split method that these subareas are created *dynamically*, because we always determine the current ion concentration at the checkpoint and the current maximum global concentration in the simulation area. Therefore our approach is a *self-adaptive* algorithm because more split points are defined at areas with unsatisfying statistical accuracy. Additional trajectory branches are suppressed, if an ion moves from lower to higher local concentration levels. Among others these features of the algorithm ensure the considerable speed-up of the Monte Carlo simulation of ion implantation into crystalline targets.

It should be mentioned that our new strategy is also best suited to compute the collision cascade of a displaced target atom ("recoil"). Depending on the ion energy and the atomic mass ratio of the ion and the recoil some collisions cause a considerable number of recoils which lead to a statistical "over-representation" of such events. The new method offers the possibility to optimize the recoil statistic by a random deletion of recoil trajectories at such places and by splitting them at peripheral areas of the collision cascade.

The trajectory split approach has been implemented in the two and three-dimensional Monte Carlo implantation module (MCIMPL) of the VISTA framework [4]. This module uses advanced physical models [5] for calculation of ion implantation into crystalline silicon, therefore it is capable of predicting 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 and material detection, an octree is used for geometry discretization [8], [9]. From our experience, geometry checks, based on such hierarchical tree representation, have no major influence on the computation time. As a typical two-dimensional technology-related example, we perform a Monte Carlo simulation of a phosphorus implant into silicon at 50 keV to obtain point response distributions. The required computational effort for such a simulation is about 1 h for the conventional approach and 17 min for the trajectory split method using a HP 735/100 workstation. The time required to perform a simulation of ion implantation into an *arbitrary three-dimensional* structure is approximately proportional to the exposed area. Typical CPU time for a three-dimensional application amounts to about 100 h using the standard method and a quarter of this time using the new simulation strategy.

III. SIMULATION RESULTS

Several simulation results presented below demonstrate the merits and applicability of the new simulation strategy. The examples in Fig. 2 show two-dimensional point-responses of phosphorus implants. We calculated distributions of phosphorus ions implanted at 50 keV, with a dose of $3 \cdot 10^{13}$ cm^{-2} through a 10-nm wide window into (100) oriented crystalline silicon covered by 2.5 nm of oxide. The beam was tilted for $8°$ in the xz-plane shown in Fig. 2 and rotated around the z-axis by $18°$ [10]. We used the conventional trajectory simulation as well as the trajectory split method in these simulations to observe and to quantify the statistical accuracy of both approaches. Fig. 2(a) shows the phosphorus distribution obtained by using the conventional Monte Carlo strategy, Fig. 2(b) presents the dopant concentration calculated by the trajectory split method. For both simulations we used 5000 distinct ion trajectories.

In order to get a reference distribution, we performed a conventional simulation run with such a high number of ion trajectories (1 000 000) that statistical fluctuations are negligible in the concentration area considered [Fig. 2(c)]. The major feature of this distribution is a pronounced peak in [001] direction due to axial channeling. Another preferential direction of the ion penetration is along the ion beam. Thus, the distribution has an asymmetric shape.

The distributions calculated with 5000 ion trajectories exhibit noticeable statistical noise. Even at this low number of simulated ions, the trajectory split method reproduces the main properties of the reference profile. Additionally,
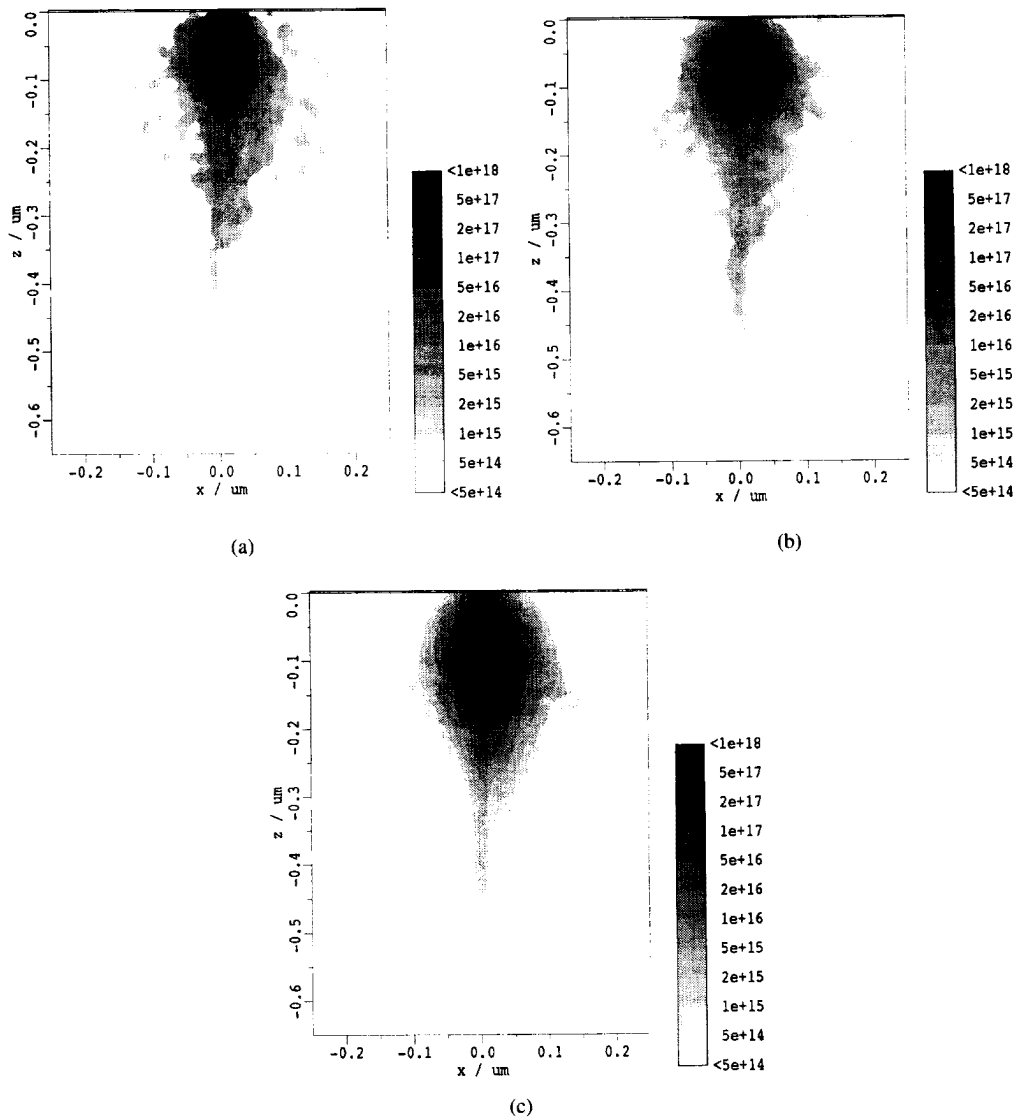
Fig. 2. Two-dimensional point responses of phosphorus implants. (a) 5000 distinct ion trajectories, conventional strategy. (b) 5000 distinct ion trajectories, trajectory split method. (c) Reference distribution: 1 000 000 ion trajectories, conventional strategy.
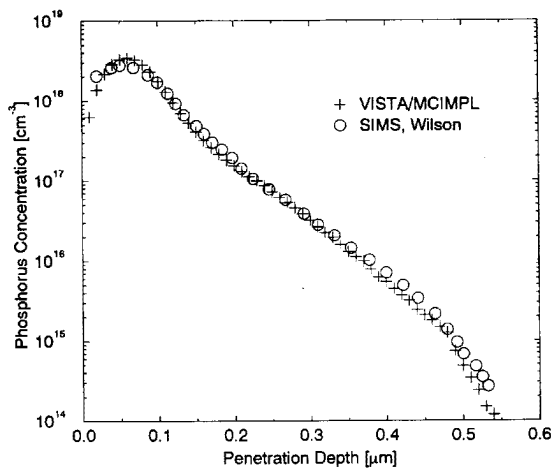

Fig. 3. Comparison between SIMS measurement and VISTA simulation.

In order to verify the results of our simulations we transformed the two-dimensional reference distribution [Fig. 2(c)] to a one-dimensional profile by means of integration along the lateral coordinate. This profile is shown in Fig. 3, where a VISTA/MCIMPL simulation result is compared to SIMS measurement of [10]. The channeling tail of the experimental profile is very well reproduced by the simulation. This is a consequence of an exactly-calibrated local electronic stopping power model for phosphorus ions in crystalline silicon. This electronic energy loss ΔE_e is a function of the ion impact parameter p and is proportional to the path length ΔR along the trajectory [5]

$$\Delta E_e(p) = S_e \Delta R \left(x_{nl} N + x_{loc} \frac{1}{2\pi a^2} e^{-\frac{p}{a}} \right) \qquad (1)$$

where S_e denotes the random electronic stopping power for a amorphous material, N is the atomic density of silicon and a is the effective screening length of the interatomic potential.
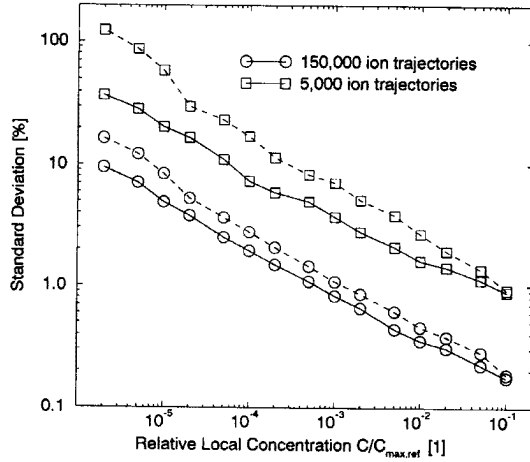
the distribution of Fig. 2(b) is smoother compared to the conventional simulation [Fig. 2(a)].

Fig. 4. Standard deviation versus relative local concentration. Dashed line: conventional method; solid line: trajectory split method.

Fig. 5. Number of ion trajectories versus standard deviation. Dashed line: conventional method; solid line: trajectory split method.

x_{nl} and x_{loc} are the nonlocal and the local fraction of S_e, respectively.

We use the following values to calculate $\Delta E_e(p)$ of phosphorus ions:

$$S_e = 1.3 S_e^L$$

where S_e^L denotes the electronic stopping power according to Lindhard [11]

$$a = 0.55 a_{Oen}$$

where a_{Oen} is the screening length proposed by Oen and Robinson [12]

$$x_{loc} = \max\left\{0, \left(1 - 0.25 \frac{E}{E_{ref}}^{0.05}\right)\right\}$$

where E_{ref} is 1 keV

$$x_{nl} = 1 - x_{loc} + x_{loc}(1 - p_{max})e^{\frac{-p_{max}}{a}}$$

where p_{max} means the maximum impact parameter used in the simulation.

To assess the statistical accuracy of the results obtained from the conventional and from the trajectory split methods, we defined the following mean-square deviation from our reference distribution Fig. 2(c):

$$\varepsilon(C) = \frac{1}{V_{ref}} \int_{C_{loc,ref} \in [C, C_{up}]} \left(\frac{C_{loc}(\vec{r}) - C_{loc,ref}(\vec{r})}{C_{loc,ref}(\vec{r})}\right)^2 dV \tag{2}$$

$$C_{up} = 10 C \tag{3}$$

where V_{ref} denotes that volume of the reference distribution where the corresponding local concentration $C_{loc,ref}(\vec{r})$ is within the interval $[C, C_{up}]$. Fig. 4 shows the mean-square deviation calculated according to (2) for two-dimensional phosphorus distributions simulated with the conventional and the trajectory split methods. We present the deviation data for
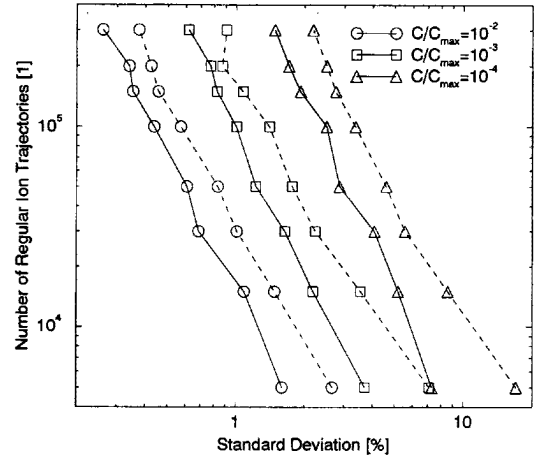
these distributions calculated with 5000 and 150 000 distinct ion trajectories.

The relative concentration shown in Fig. 4 is defined as the ratio of $C/C_{max,ref}$, where $C_{max,ref}$ means the maximum concentration of the reference distribution. It is evident that the relative standard deviation decreases for high local concentrations. Therefore, areas with low local concentration are well suited to demonstrate the merits of the new simulation strategy. A conspicuous difference between the conventional and the trajectory split method is obtained at low local concentration and small number of ion trajectories. Our strategy shows a deviation from the reference distribution which is up to four times smaller compared to the standard result.

Another advantage of the trajectory split method is its lower sensitivity to the local concentration. The mean-square error in a conventional simulation (5000 ion trajectories) increases by a factor of 2.8 per decade of concentration decrease, whereas this factor is only 2.0 per decade for the trajectory split method. It is desirable to minimize the error sensitivity to local concentration and the trajectory split method offers this capability by performing more than one split at each split point.

The computation time for Monte Carlo simulation of ion implantation is a crucial aspect of practical applicability. To demonstrate the effect of the new simulation strategy on the calculation time, we present the results of 16 simulation runs performed with both methods using different numbers of distinct ion trajectories. Fig. 5 shows the number of ion trajectories required to achieve a given relative standard deviation at a specified concentration level. The critical simulation errors are associated with low concentrations. To obtain a simulation result where the relative local concentration at 10^{-4} deviates 5% from the reference distribution we need 40 000 distinct ion trajectories for the conventional strategy and on the other hand only one third of this number for the new method, see Fig. 5). Fig. 6 shows the two-dimensional point-response obtained from the trajectory split method for 15 000 calculated trajectories. The computational effort is approximately proportional to the number of distinct ion
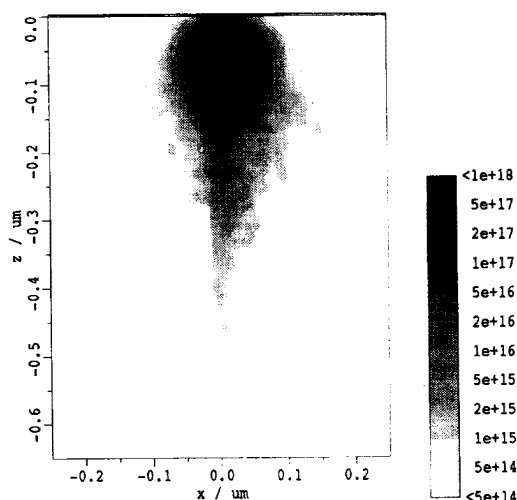
Fig. 6. Two-dimensional point response of a phosphorus implant calculated with 15 000 distinct ion trajectories, trajectory split method, satisfying statistical accuracy.

trajectories and the additional overhead due to trajectory splits is about 10–25%.

It should be mentioned that 5% deviation in concentration only means 0.3% error in prediction of penetration depth at this concentration (see Fig. 3), which is sufficient for practical purposes. Expressed in absolute values, the relative concentration of 10^{-4} in Fig. 5 is equivalent to an absolute concentration of 10^{15} cm^{-3} at a depth of 0.5 μm in Fig. 3.

IV. CONCLUSION

A new method for Monte Carlo simulation of ion implantation which is applicable to arbitrary two- and three-dimensional geometries is presented. A continuous comparison between local and maximum global concentration is applied in our simulation strategy. The simulation area is dynamically divided into layers each representing a certain relative concentration level of the calculated distribution. Each ion trajectory is traced and split into several virtual branches in cases 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 concentration. As a result, the time required to perform a simulation with comparable statistical accuracy is reduced typically by a factor of three to five in comparison to the standard approach.

It follows from the quantitative analysis of statistical accuracy that our approach has potential for further optimization. Especially the optimum number of virtual branches with respect to the dimension of the problem will be investigated and further methods, which allow recursive splitting, will be developed.

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