Adaptive Grid for Monte Carlo Simulation of Ion Implantation

H. Stippel[1], S. Halama[1], G. Hobler[2], K. Wimmer[1] and S. Selberherr[1]
[1]*Institute for Microelectronics*
[2]*Institute für Allgemeine Elektrotechnik und Elektronik*
Technical University Vienna, Gusshausstrasse 27-29, A-1040 Vienna, Austria/EUROPE

Abstract

An automatic grid design and adaption algorithm for Monte Carlo simulation of Ion Implantation (MCI^2) has been developed. This method has been successfully implemented in the two-dimensional process simulator PROMIS. Based on range parameters a dense initial grid is designed. Dose conservation and gradient resolution criteria are used to determine gridlines which can be deleted. Special attention has been focused on a homogenous variation of the grid spacing. The implemented algorithm produces a suitable grid for the resolution of implanted profiles, and can be successfully applied to the three-dimensional case.

1 Motivation

In recent years several methods have been developed to improve the performance of multi-dimensional Monte Carlo simulation tools for Ion Implantation [1], [2], [3]. These improvements, and the performance of today's workstations have resulted in feasible CPU-times. One shortcoming for the everyday use of MCI^2 tools, however, is the lack of an automatic grid design.

The manual generation of a suitably refined grid for MCI^2 simulations, besides being a tedious and time-consuming task, becomes virtually impossible in three dimensions. Non-adaptive grid generators on the other hand, in which the mesh does not mirror the expected implanted ion distribution, may yield grids which are either too sparse to guarantee the desired resolution, or so dense that statistical noise poses a significant threat to the accuracy of the result.

In all other parts (e.g. analytic ion implantation, diffusion) of our process simulator PROMIS [4], automatic grid generation and adaption had already existed. A new adaption technique has been implemented for the MCI^2 of PROMIS in order to totally free the user from any need to define a grid manually.

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2 Grid Adaption Criteria

The criterion used for the grid adaption algorithm depends on both the integral of the dose error IDE along the gridline (e.g. [4], [6]) and the maximum concentration gradient GDC, which are calculated at every point in the grid. The dose conservation criterion outlined in (1) minimizes the local dose error, whereas the gradient criterion (2) which is applied to the logarithm of the concentration guarantees a good resolution of steep gradients in the dopant profile. In (1), (2), (3), (4) the criteria are formulated for gridline i at $x = x_i$. To obtain the corresponding criterion for gridline j at $y = y_j$ one only has to exchange x and y and i and j, respectively.

$$IDE_i = \sum_{j=1}^{n_j} \frac{1}{12} \cdot \Delta x_i^3 \cdot \Delta y_j \cdot \left(\frac{\partial^2 C(x,y)}{\partial x^2} \right)_{i,j} \tag{1}$$

$$GDC_i = \max_j \left(\left| \frac{C_{i+\frac{1}{2},j}}{C_{i-\frac{1}{2},j}} \right|, \left| \frac{C_{i-\frac{1}{2},j}}{C_{i+\frac{1}{2},j}} \right| \right) \tag{2}$$

Then the maximum of the two criteria is determined, resulting in a measure I_i for the importance of the line i (3).

$$I_i = \max(IDE_i, GDC_i) \tag{3}$$

Subsequently, the line having the smallest total criterion is determined, provided its removal does not violate a certain distance ratio between neighboring lines (4). This grid line is deleted.

$$x_{i+1} - x_{i-1} \leq K \cdot \min(x_{i+2} - x_{i+1}, x_{i-1} - x_{i-2}) \tag{4}$$

It is to be noted that the term $\left(\frac{\partial^2 C(x,y)}{\partial x^2} \right)_{i,j}$ in equation (1) is not the discretization of the second partial derivative of the function $C(x,y)$ with respect to x. It is only a short form for the second difference quotient.

$$\left(\frac{\partial^2 C(x,y)}{\partial x^2} \right)_{i,j} \doteq 2 \cdot \frac{C_{i+1,j} \cdot (x_i - x_{i-1}) + C_{i-1,j} \cdot (x_{i+1} - x_i) - C_{i,j} \cdot (x_{i+1} - x_{i-1})}{(x_{i+1} - x_i) \cdot (x_i - x_{i-1}) \cdot (x_{i+1} - x_{i-1})} \tag{5}$$

There is a slight difference between the gradient (GDC) and the dose conservation criterion (IDE). In (5) $C_{i,j}$ is the concentration on the gridpoint i,j, whereas in (2) $C_{i\pm\frac{1}{2},j}$ are the concentrations in the boxes adjacent to line i.

3 The Algorithm

In PROMIS, the region of interest is initally analysed using a very dense, uniform grid, thus partitioning it into histogram-boxes (squares in two, cubes in three dimensions) whose sides are delimited by adjacent grid lines. Each time a particle comes to rest at some point $\mathcal{P}$, the particle counter of the surrounding box $B(\mathcal{P})$ is increased. Only squares with a non-zero particle count are stored. Therefore, memory requirements are reduced and access to the data is very efficient. The mapping of the stored boxes to the real box position is performed by an index table.

To find out the box where an ion stopped, that is, finding $B(\mathcal{P})$ for a given $\mathcal{P}$, a binary search is performed. This reduces the overall computation time by about 10 % in comparison to a linear search algorithm. The number of squares containing at least one particle is traced. If it exceeds a predefined allowed maximum, the least significant grid lines are removed according to the above mentioned criteria.

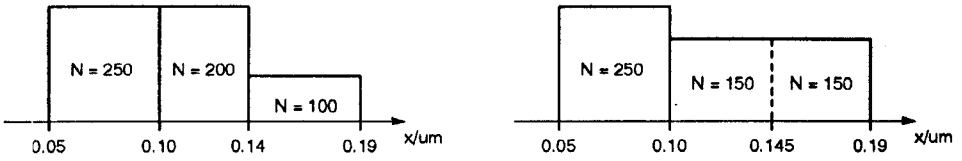

Figure 1: Drift of particles on deleting and inserting lines

In contrast to other grid adaption algorithms [5], the insertion of grid lines during the computation is forbidden, since the redistribution of the particles among the newly created boxes cannot be determined unambiguously, thus causing unintentional and unphysical drift of particles (see Fig. 1). Since gridlines can only be deleted, besides the above mentioned criteria careful investigations have to be performed if a line can be removed.

The initial grid spacing d_i in this work is related to the minimum expected lateral standard deviation σ_{LAT} in the region, to guarantee good resolution of the expected profiles. The same quantity σ_{LAT} is used to determine the subwindow size in the superposition method [2] and hence the ions' entering points. We have observed that an initial grid spacing $d_i = 0.1 \cdot \sigma_{LAT}$ maintains a satisfactory resolution, whilst this choice also restrains the number of deletion steps.

If box entries in the table containing the stored boxes have to be deleted due to memory overflow, grid lines have to be deleted. The neighboring boxes separated by this line are combined (see Fig. 2 and Fig. 3) and the corresponding particle numbers added. In this case the box index table is changed consistently.

Typically, during the first adaption passes the only grid lines which are deleted are those which delimit empty boxes. If they are deleted, the memory requirements are not reduced and the algorithm has to be performed a second time. Consequently, we get some regions with very large boxes compared to others. Later on in the simulation, if any particle stops in one of the larger boxes, a noticeable error in the final profile is caused, as the concentration is computed from the number of particles in a rectangle weighted by the box size. The condition (4) guarantees a mostly homogenous box size and, additionally, the number of

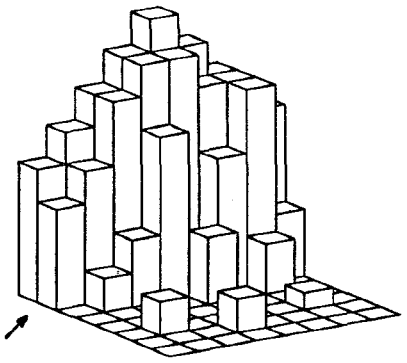

Figure 2: Histogram before deletion

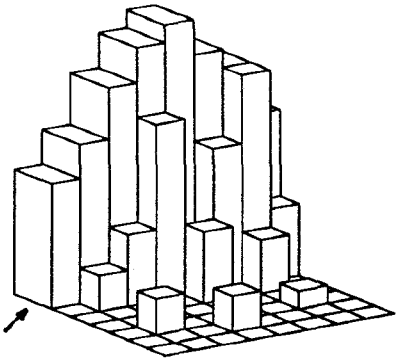

Figure 3: Histogram after deletion

deletion steps (grid updates) is minimized. This also reduces the total computation time.

4 Examples

The effect of the grid adaption algorithm shall be demonstrated by simulations of a boron implantation into a simple masked (SiO_2) silicon wafer (tilt angle 0^o, implantation energy 100 keV). The same implantation has been performed twice, both starting with the same initial grid. The final implanted distributions for a computation performed without grid adaption, and using the adaption method are shown in Fig. 4 and Fig. 5, respectively. The first example (Fig. 4) uses 10404 boxes (10609 nodes) the second one (Fig. 5) allows a maximum of 500 stored boxes; the resulting grid contains 2205 nodes. It is to be noted that the grid adaption generates a grid which is as coarse as possible, but still sufficiently fine to reproduce the doping profile properly. Therefore the statistical noise is implicitly reduced.

5 Conclusion

An automatic grid generation and adaption algorithm for MCI[2] has been presented. In contrast to other grid adaption algorithms special considerations have been taken into account to guarantee a mostly homogenous grid. Our investigations have shown that this method produces a suitable grid, despite the later occurence of some statistical spread. A two-dimensional version of this algorithm has been implemented in the process simulator PROMIS. An extension to the three-dimensional case appears to be a straightforward task. As only histogram-boxes containing at least one particle are stored ($B(\mathcal{P}) \neq 0$), memory requirements are greatly reduced.

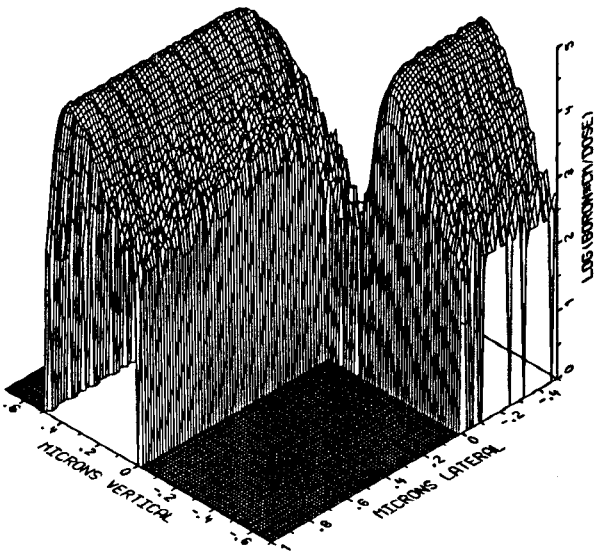

Figure 4: Boron implantation without grid adaption

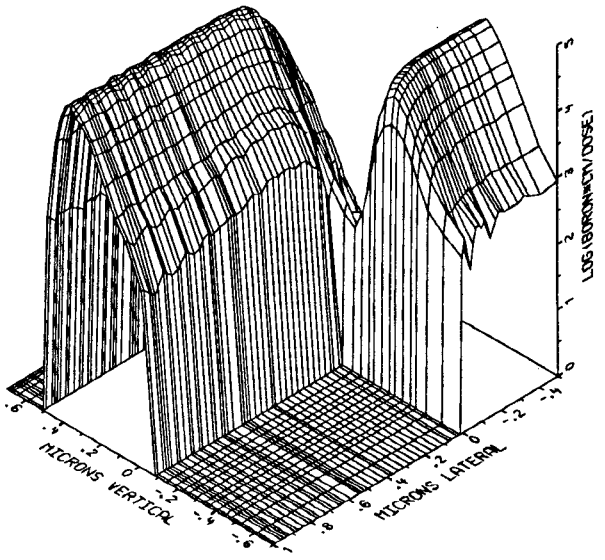

Figure 5: Boron implantation with grid adaption

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