Two Methods to Improve the Performance of Monte Carlo Simulations of Ion Implantation in Amorphous Targets

EDDIE VAN SCHIE AND JAN MIDDELHOEK

Abstract—**This paper describes two methods to improve the results of a Monte Carlo technique to simulate the transport of energetic ions in amorphous targets in two dimensions. The target considered is a homogeneous monolayer. The Monte Carlo technique used is based on the program TRIM [5], [6]. The first method relies on the fact that some calculated data can be used more than once. The second method relies on the fact that a point source results in a rotation-symmetric ion distribution. To study the behavior of the two methods a smoothness indicator has been defined. It is a measure for the distance of a simulation result to the ideal result, i.e., the result based on an infinite number of ion trajectories. This indicator showed that a CPU time reduction of a factor 80 has been achieved.**

I. Introduction

DEVELOPMENT of advanced VLSI processes requires detailed modeling of each stage of the total fabrication process to predict device geometry and impurity profiles and to provide the input for device simulation programs. Ion implantation is the primary method for introducing dopants into semiconductors. The control over the particular dopants as well as over the energy and dose has made implantation an indispensable tool for the fabrication of micron and submicron structures. Especially for submicron processes detailed understanding of the implantation process in two or three dimensions is required. Modeling inaccuracies which in the past remained hidden by extended thermal treatments, can now cause significant differences between theory and experiment.

Ion implantation is the introduction of accelerated ionized atoms into targets with kinetic energies up to about 1000 keV. An individual implanted ion undergoes scattering events with electrons and atoms of the target, reducing the ion's kinetic energy until it comes to rest. The scattering of the ion with the target atoms causes a change in the direction of motion of the ion, resulting in a lateral straggling of the ion distribution. For small device geometries needed in VLSI applications, the lateral ion straggling effects become extremely important. In MOS transistors the lateral ion straggle of the source and drain implantation is a limiting fundamental factor determining the doping between source and drain and the electrical channel length.

Two calculation strategies exist for modeling implantation in two dimensions. In the first strategy the ion beam is viewed as the summation of infinitesimal thin ion beams. The two-dimensional distribution of such a thin ion beam can "easily" be calculated. This distribution is called a line source response function (LSR) because a two-dimensional distribution is the result of a line source. In the second strategy the calculations are performed over the full width of the target. It is clear that the second strategy consumes much CPU time.

In the present work the LSR is calculated by means of a Monte Carlo method in a layer of amorphous silicon. The results which are obtained by Monte Carlo simulations are quite noisy and require much CPU time. This can be overcome by using a large number of simulated ions or using a coarse discretization of the simulation area. The first solution increases the CPU time. The last solution decreases the obtained resolution. Some methods exist to improve the results of a Monte Carlo simulation. Giles [1] used projections on the depth axis and lateral axis. However for high energies this appears to be inappropriate since then the lateral spread is a function of the depth [2]. Albers [3] used the fact that a two-dimensional distribution is symmetric. Petersen [4] performed calculations on a supercomputer. In this paper two methods are introduced to improve the performance of the Monte Carlo results. Our computer code is based on the program TRIM [5], [6]. A summary of this code is given in Section II. In Section III both methods will be introduced. In Section IV results are analyzed and discussed. In Section V an example is shown. In Section VI the conclusions are summarized.

II. The TRIM Monte Carlo Code

As with other Monte Carlo programs, the method consists of following a large number of individual ion trajectories in a target. Each history begins with a given energy, position and direction. There are two basic assumptions made in the program TRIM [5]. The first one is that the ion does not sense any crystallographic order in the target, i.e., the target is amorphous. In practice this is achieved by tilting the target away from open crystallographic axes.

Manuscript received February 23, 1988; revised May 5, 1988 and September 13, 1988. This work was supported by the National Innovative Research Project under IOP IC-TEL 45.013. The review of this paper was arranged by Associate Editor W. Fichtner.

The authors are with the IC Technology and Electronics Group, University of Twente, 7500 AE Enschede, The Netherlands.

IEEE Log Number 8824850.

The second one is that a particle is assumed to change direction as a result of nuclear collisions and to move in straight free-flight paths between collisions. The energy is reduced as a result of (elastic) nuclear collisions and an (inelastic) electron gas energy loss. Both loss mechanisms are assumed to be independent.

The typical sequence of calculating the motion of an ion is as follows. The ion is assumed to be incident from the top surface of the target. Given this direction, position and the starting energy an impact parameter p is selected randomly. The nuclear energy loss and scatter angle are calculated using the functional approximation of the scattering integral according to Biersack [6]. To be able to calculate new coordinates, a random azimuthal angle ϕ is also needed: $\phi = 2\pi\xi$ where $\xi \in \langle 0, 1 \rangle$ is a random number. The average free-flight path length between collisions is $L = \rho^{-1/3}$ where ρ is the atomic density. For this path length L the inelastic energy loss is calculated. This electronic stopping is approximated by the energy dependent method described in [5]. Given the scatter angle, the azimuthal angle and the path length L, the new direction, position and energy of the ion can be calculated. This procedure is repeated until the ion comes to rest. An ion is considered to be stopped when its energy drops below a prespecified value or when its position is outside the target. The trajectory which has been obtained is three dimensional, as shown in Fig. 1. To obtain a LSR, this trajectory is projected into a plane. During the calculation of the trajectory the position of the ion is tracked in this two-dimensional plane.

During a simulation many ion trajectories are calculated. The coordinates of the positions where the ions stop are stored in a histogram. This corresponds to a two-dimensional discretized target as shown in Fig. 1. A cell element i, j with position:

$$y_i = (i - 1)\,\Delta Y$$
$$z_j = (j - 1)\,\Delta Z \tag{1a}$$

is defined by the cell boundaries:

$$(i - 1 - \tfrac{1}{2})\,\Delta Y \le y < (i - 1 + \tfrac{1}{2})\,\Delta Y$$
$$(j - 1 - \tfrac{1}{2})\,\Delta Z \le z < (j - 1 + \tfrac{1}{2})\,\Delta Z. \tag{1b}$$

If an ion stops in cell i, j then the histogram is adapted as

$$H_{i,j} := H_{i,j} + 1. \tag{2}$$

The related probability function is then

$$F_{i,j} = H_{i,j}/N. \tag{3}$$

where N is the number of calculated trajectories. The obtained histogram can be used to calculate a two-dimensional impurity distribution under an arbitrarily shaped mask edge [1], [2], [4], [7]–[9].

III. Description of the Methods

Two methods to improve the results of the previously described Monte Carlo method are now presented. The first method is based on the fact that certain calculated values during the evolution of one ion trajectory can be used more than once. The second method is based on the fact that the formulation using a point source response is rotationally symmetric.

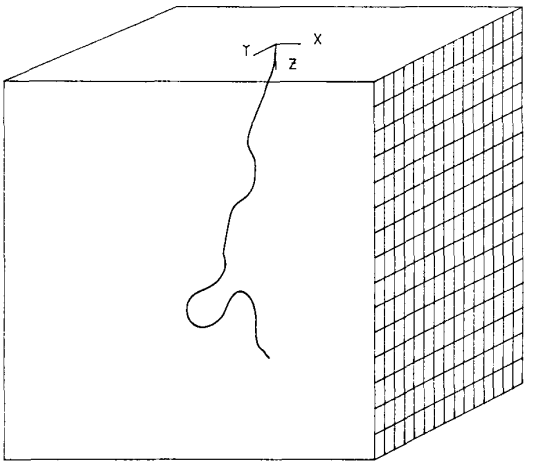


Fig. 1. Projection of a three-dimensional ion trajectory on a discretized yz-plane.

A. Identical Energy Histories

During a collision several values have to be calculated. Among them are:

1) the scatter angle and energy loss using a randomly selected impact parameter.
2) the electronic energy loss during the movement over a distance L.
3) the new coordinates given the scatter angle, a random selected azimuthal angle and the distance L.

The azimuthal angle does not influence the energy transfer of a collision but only the direction of the ion after a collision. So the third calculation may be performed M times to obtain different ion trajectories in space, which have identical energy loss sequences during the movement of the ions.

A question to be considered is how large M can be chosen. There are two constraints concerning this choice. The first constraint is that these M trajectories will be related in some sense, i.e., it will be impossible to obtain a correct Monte Carlo result when only one energy loss sequence is calculated and for instance $M = 10^4$ is used. In Fig. 2 some trajectories are plotted for a Boron implant at 20 keV. The horizontal axis corresponds with the distance R between the position of the ion and the beam axis. The vertical axis corresponds with the depth z of the ion. In Fig. 2(a) 10 trajectories are plotted based on 10 different energy loss sequences. In Fig. 2(b) 10 trajectories are plotted based on only one energy loss sequence. A comparison of both types of trajectories reveals a certain relation between trajectories based on the same energy loss sequence. This is an indication that one energy loss sequence cannot be used too often. Although it is difficult

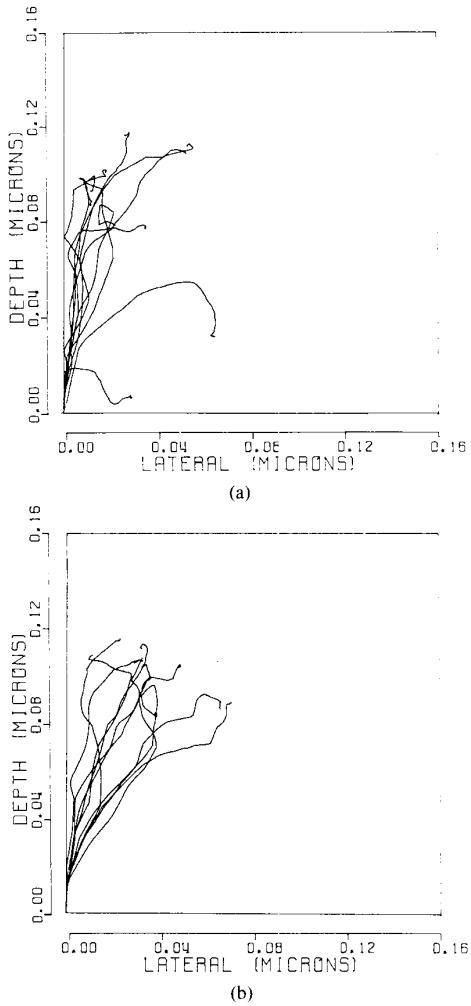


Fig. 2. (a) 10 boron trajectories calculated with 10 energy sequences. (b) 10 boron trajectories calculated with only 1 energy sequence.

to prove analytically, a large number of simulations showed that this effect has a minor influence on the LSR when N is large and $M << N$.

The second constraint is given by the estimated saving in CPU time. The CPU time of the calculation of one ion trajectory can be split into two parts: α, the average CPU time spent to calculate energy losses and β, the average CPU time spent to calculate coordinates. The total CPU time to calculate N_1 different ion trajectories is thus given by

$$T_1 = \alpha N_1 + \beta N_1. \tag{4}$$

Another way to obtain N_1 trajectories is to calculate N_2 energy loss sequences and use them M times to obtain $N_1 = N_2 M$ trajectories. The CPU time is then given by

$$T_2 = \alpha N_2 + \beta N_1 = N_1(\alpha/M + \beta). \tag{5}$$

The reduction in CPU time is given by the quotient of (4) and (5):

$$q = \frac{T_2}{T_1} = \frac{1 + (\alpha/\beta)/M}{1 + (\alpha/\beta)}. \tag{6}$$

So the CPU time reduction is limited by

$$q_{\text{lim}} = \frac{1}{1 + (\alpha/\beta)}. \tag{7}$$

In the used computer code the ratio α/β roughly equals 3, so $q_{\text{lim}} = 1/4$. Choosing $M = 10$ results in a CPU time reduction of $1/3.9$. Increasing M above 10 does not lead to a significant reduction of CPU time.

B. Rotation Symmetry

In the conventional Monte Carlo technique in two dimensions, the three coordinate axes x, y, z are chosen at the beginning of the simulation and all ion trajectories are projected into one plane, for instance the yz plane. This plane is identical with the discretized sidewall of the cube in Fig. 1. However this choice is arbitrary. If the cube in Fig. 1 is rotated the ion trajectory does not change but the projection on the sidewall changes. Thus using one set of three-dimensional trajectories gives rise to different two-dimensional projections, which is an indication that the data set is not used efficiently. This is caused by the fact that the result of a Point Source should be rotationally symmetric. A three-dimensional histogram in a three-dimensional discretized space will not be rotationally symmetric using the data set. To force this three-dimensional histogram to be rotationally symmetric one could rotate each trajectory. This can be considered to be equivalent with the choice of an infinite number of azimuthal angles for the first collision.

The mathematical treatment depends on the interpretation but gives identical results. Firstly, one could store several histograms each corresponding with a projection in a rotated plane. From these histograms an average histogram can be calculated which will be smoother than a single histogram. It is possible to derive an analytical expression to update the average histogram of an infinite number of rotated planes after the calculation of a single three-dimensional trajectory. Secondly, one could store a radial histogram and project it on a plane after the calculation of all the three-dimensional trajectories. Finally one gets the most simple treatment if each three-dimensional trajectory is rotated and projected in the plane of Fig. 1.

Consider an ion trajectory with end point coordinates x_p, y_p, z_p. In the xy plane a circle C with radius R_p can be drawn through the points x_p, y_p around the beam axis. Imagine that this trajectory is rotated Q times with rotation angle $\Delta\zeta$.

$$\Delta\zeta = 2\pi/Q. \tag{8}$$

Thus Q trajectories are obtained all having their endpoints on the circle C. If these trajectories are projected into the yz plane of Fig. 1, a cell with y index i will get P_i ions, with P_i about:

$$P_i = 2(\zeta_{i-1/2} - \zeta_{i+1/2})/\Delta\zeta \tag{9}$$

where $\zeta_{i-1/2}$ is the angle between the x-axis and the intersection between the cell boundary $y_{i-1/2}$ and the circle C. Now the weight function $W_i(R_p)$ is defined:

$$W_i(R_p) = P_i/Q$$

which evaluates to

$$W_i(R_p) = \frac{1}{\pi}\left[\arccos\left(\frac{y_{i-1/2}}{R_p}\right) - \arccos\left(\frac{y_{i+1/2}}{R_p}\right)\right]. \tag{10}$$

Note that for $y_{i+1/2} > R_p$ one should use $y_{i+1/2}/R_p = 1$ and for $y_{i-1/2} < -R_p$ one should use $y_{i-1/2}/R_p = -1$.

To update the histogram after the calculation of a trajectory (1) is replaced by

$$H_{i,j} := H_{i,j} + W_i(R_p) \tag{11}$$

for all the cells i if the ion stops at cell depth j with a radius R_p.

IV. Analysis of the Results

To study the behavior of the methods it is checked whether usage of the methods speeds up the convergence to the final solution. The final solution is the probability function F based on an infinite number of trajectories. The following error definitions are introduced:

$$e^2_{\text{abs}} = \frac{1}{N_{\text{cells}}}\sum_{i,j}\left(10^5 \cdot F_{i,j} - 10^5 \cdot F^{\infty}_{i,j}\right)^2 \tag{12a}$$

$$e^2_{\text{rel}} = \frac{1}{N_{\text{cells}}}\sum_{i,j}\left(\frac{10^5 \cdot F_{i,j} - 10^5 \cdot F^{\infty}_{i,j}}{\max\left(1,\ 10^5 \cdot F^{\infty}_{i,j}\right)}\right)^2 \tag{12b}$$

where $F^{\infty}_{i,j}$ represents the histogram for $N = \infty$. The factor 10^5 is used to transform the results as if they were histograms constructed out of 10^5 ions. With this error measure one can check: a) how far a solution is from the final solution and b) if there exist some systematical error.

The problem is that the final solution has to be calculated first before this error measure can be calculated. The function $F^{\infty}_{i,j}$ is represented by a fit function for the purpose of this study. The form of the function is

$$F^{\infty}_{i,j} = k \cdot f_{\text{dep}}(z) \cdot f_{\text{lat}}(z, y). \tag{13}$$

The function f_{lat} represents the lateral spread. It is a function of the depth and is given by

$$f_{\text{lat}}(z, y) = c(z) \cdot e^{-|b(z)\cdot y|^{p(z)}}. \tag{14}$$

This function has been introduced by Hobler *et al.* [2]. In [2] also some parametrized functions for $c(z)$, $b(z)$ and $p(z)$ are given. For $f_{\text{dep}}(z)$ some well known alternatives are available such as Pearson IV, Gaussian and double sided Gaussian. For the present study however none of these functions fitted the Monte Carlo data good enough. A splitted pseudo-Gaussian is used

$$f_{\text{dep}}(z) = e^{-a1|z|^{p1}}, \quad z \le z_{\text{split}}$$
$$f_{\text{dep}}(z) = e^{-a2|z|^{p2}}, \quad z > z_{\text{split}}. \tag{15}$$

All the fit parameters are obtained by means of the flexible parameter extractor PROMEA [10].

The obtained results are presented in an example for a boron implant of 20 keV. The yz-plane is discretized with $\Delta Z = \Delta Y = 16$ Angström. The method based on multiple use of energy sequences uses $M = 10$. In Fig. 3 some contours of the result using both methods are plotted (dotted line) and when none of the methods is used (drawn line). Because the LSR is symmetric only one half is shown. The result with no special method is calculated with a coarser discretization, because otherwise the figure would contain too much noise. The histogram of Fig. 3 is used to obtain the fit parameters. The result of the fit is shown in Fig. 4.

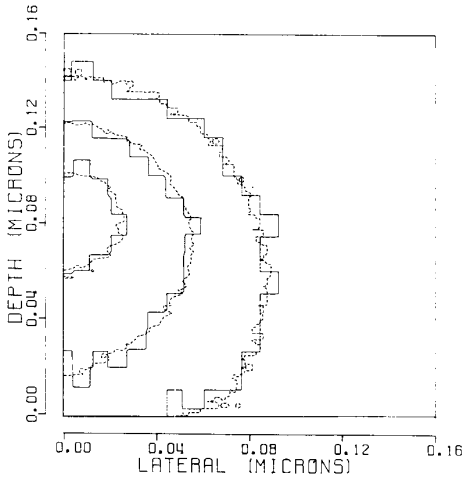


Fig. 3. The dotted line is a contour plot of the histogram based on N = 10.000 energy sequences which are M = 10 times used and with rotation symmetry. The drawn line is a contour plot of the histogram based on N = 10.000 energy sequences which are now M = 1 times used and without rotation symmetry.

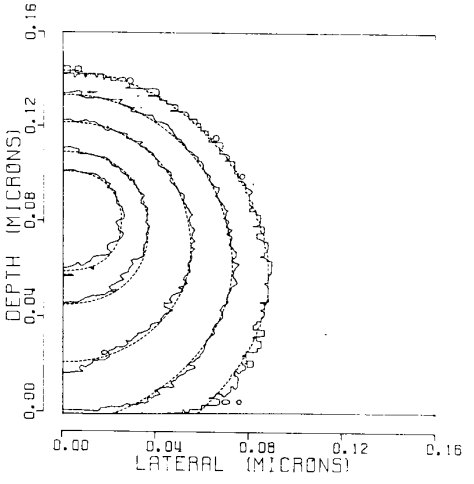


Fig. 4. The result of the fitting procedure. The dotted lines are the fit results, the drawn lines are the *MC* results.

Values of the fit errors given by (12a) and (12b) as function of the number of calculated trajectories, found after repeating the calculations are shown in Fig. 5. The error estimates of four histograms are shown:

1) the result when none of the methods is applied,

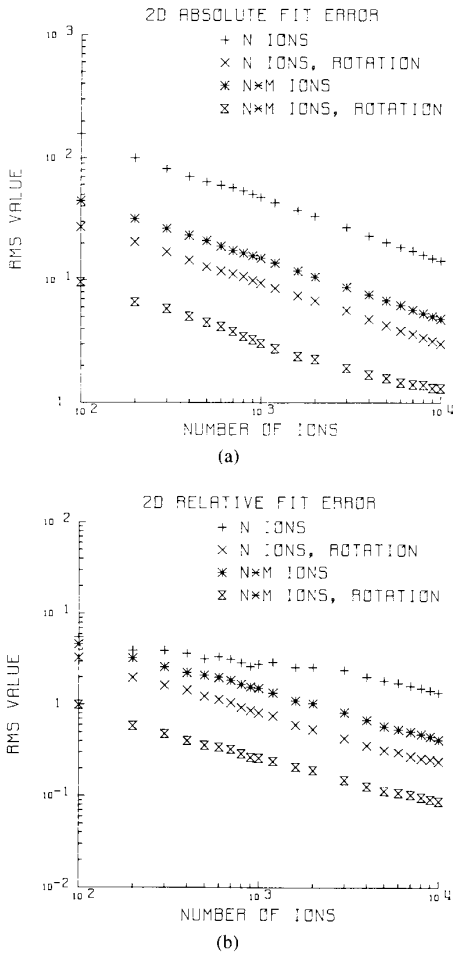


Fig. 5. Error estimates as a function of the number of simulated ions (a) the absolute error estimates. (b) the relative error estimates.

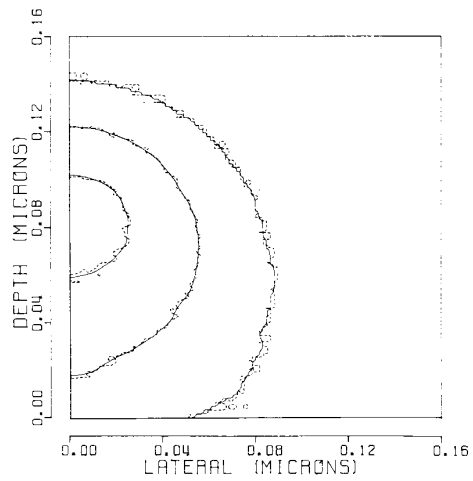


Fig. 6. Results of the smoothing operation. The drawn line is the smoothed histogram, the dotted line is the original.

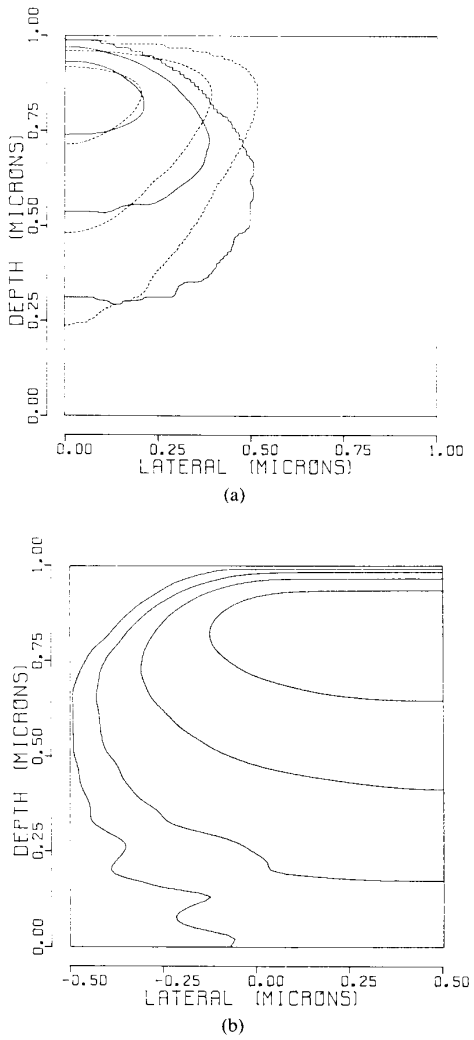


Fig. 7. (a) Contour plot of a boron implant of 300 keV. The drawn line is the correct Monte Carlo result. The dotted line is a reconstruction out of the projections on the depth axis and the lateral axis, simulating a constant lateral straggle. (b) Profile under an infinite steep mask edge with an implantation dose of 10^{14} ions/cm^2. The shown levels are 10^{15}, 10^{16}, 10^{17}, and 10^{18} ions/cm^3.

2) only rotation symmetry is applied,
3) only identical energy histories are used with $M = 10$,
4) both methods are used.

For the fourth histogram it can be seen that the error is limited by the "systematical" fit error. If we ignore this and draw straight lines through the points we see an almost parallel behavior of the curves. The horizontal shift from histogram 1 to histogram 3 and from histogram 2 to histogram 4 indicates that a value $M = 10$ indeed reduces the number of required ions with a factor of 10. In terms of cpu time this factor is about 4. The horizontal shift from histogram 1 to histogram 2 and from histogram 3 to

histogram 4 indicates that the number of required ions reduces with a factor of 20. In terms of cpu time this is also a factor 20. The conclusion is that the use of both methods reduces the cpu time with a factor of 80 to obtain a result with the same error level as a calculation where no methods are applied.

V. An Example

To demonstrate the capabilities of the computer code a boron implant of 300 kev is simulated. The characterization of the simulation is $N = 2000$, $M = 10$, $\Delta Z = \Delta Y = 100$ Angstrom, rotation symmetry is used. To smooth the obtained results the following algorithm is applied. The smoothing algorithm takes the logarithmic average of a block of 9 cells as in (16):

$$F_{i,j} := \left(\prod_{l=-1}^{1} \prod_{k=-1}^{1} F_{i-l,j-k} \right)^{1/9} \qquad (16)$$

This smoothing operation is repeated 4 times. To prevent cells with zero ions to disturb the edges of the histogram, the minimum value in the histogram is searched unequal to zero. If during the smoothing a cell with value zero is encountered, this minimum value is used instead. This kind of smoothing behaves very well as can be seen in Fig. 6.

The results are shown in Fig. 7. In Fig. 7(a) the LSR is plotted (drawn line). In the same figure the LSR is shown which is the result of a reconstruction out of the projections on the vertical and horizontal axes as is done in [1], [9] (dotted line). In other words, it is assumed that the lateral straggling is not a function of the depth. For high energies it appears that this assumption is not valid, see also [2]. Only for the top of the profile the fit seems good enough. For lower energies the assumption becomes more valid, because the depth dependence of the lateral straggling is less in that case.

In Fig. 7(b) the profile under an infinite steep mask edge is plotted. The shown contours are at the levels 10^{15}, 10^{16}, 10^{17}, and 10^{18} ions/cm^3, the maximum of the profile is 5×10^{18} ions/cm^3.

III. Conclusion

Monte Carlo techniques are extremely powerful to simulate the transport of energetic ions in solids, although they suffer from the drawback of large CPU time requirements. In this paper two methods have been demonstrated which substantially diminish this problem for the calculation of the LSR in an amorphous monolayer. A CPU time reduction of a factor 80 is achieved compared to the conventional implementation to obtain results with a high resolution.

References

[1] M. D. Giles and J. F. Gibbons, "Two-Dimensional ion implantation profiles from one-dimensional projections," *J. Electrochem. Soc.*, vol. 132, p. 2476, 1985.

[2] G. Hobler, E. Langer and S. Selberherr, "Two-dimensional modeling of ion implantation with spatial moments," *Solid State Electron.*, vol. 30, no. 4, p. 445, 1987.

[3] J. Albers, "Monte Carlo simulation of one- and two-dimensional particle and damage distributions for ion-implanted dopants in silicum," *IEEE Trans. CAD*, Vol. CAD-4, no. 4, p. 374, 1985.

[4] W. P. Petersen, W. Fichtner and E. H. Grosse, "Vectorized Monte Carlo calculation for the transport of ions in amorphous targets," *IEEE Trans. Electron Dev.*, vol. ED-30, p. 1011, 1983.

[5] J. F. Ziegler, J. P. Biersack and U. Littmark, "The stopping and range of ions in solids," *The Stopping and Ranges of Ions in Matter*, New York: Pergamon, vol. 1.

[6] J. P. Biersack and L. G. Haggmark, "A Monte Carlo computer program for the transport of energetic ions in amorphous targets," *Nucl. Inst. and Methods*, vol. 174, p. 257, 1980.

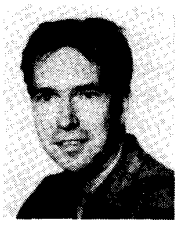
[7] S. Furukawa, H. Matsumara and H. Ishiwara, "Theoretical considerations on lateral spread of implanted ions," *Japan J. Appl. Phys.*, vol. 11, p. 134, 1972.

[8] H. Runge, "Distribution of implanted ions under arbitrarily shaped mask edges," *Phys. Stat. Sol. (A)*, vol. 39, p. 595, 1977.

[9] M. D. Giles, "Calculation of ion implantation profiles for two-dimensional process modeling," in *Simulation of Semiconductor Devices and Processes*, vol. 2, *Proc. 2nd Int. Conf.*, Swansea, July 21–23, 1986.

[10] P. B. M. Wolbert, "PROMEA: A flexible parameter extractor," M.Sc. thesis, Univ. of Twente, 1986.

*



Eddie van Schie received the M.Sc degree from the University of Twente, The Netherlands, in 1985.

In 1986 he joined the laboratory for Integrated Circuits at the University of Twente to build up a process and device simulation system. He was a visiting scientist at the Philips Research Laboratories Sunnyvale, USA, from September 1987 to December 1987. His current research interests are the development of CAD tools for process simulation and verification methods for model parameters.

*

Jan Middelhoek received the M.Sc. degree from the Free University, Amsterdam, and the D.Sc. degree from the State University, Leiden, The Netherlands.

He is a professor at the University of Twente in the Netherlands, where he teaches IC. technology and Electronics. His research is concentrated on the applications of MeV ion implantation in IC fabrication and he is head of the Laboratory for Integrated Circuits.

Dr. Middelhoek is a member of the German/Dutch MEGA expert committee for the development of submicron-technology.