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

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SUMMARY 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 a fast analytical and the Monte-Carlo simulation method.

key words: *ion implantation, three-dimensional, Monte-Carlo, analytical, simulation*

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 at least as good as 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 was 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 yields good results for many applications. Normally Gaussian, Pearson, Double Pearson, or Pearson functions with an exponential tail are used to model the point response distribution [1], [2]. Because of robust and efficient algorithms [3], [4] implemented, the important advantage of the analytical simulation methods is their 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 using experimental results for the process window in question before they can be applied to specific problems.

On the other hand side 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 traced 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 quality of the models that describe the physical behavior. These models are applicable for a wider range of implantation conditions without additional calibration [5], [6]. To achieve the same statistical accuracy of three-dimensional simulations as in two dimensions, the number of ions traced must be considerably increased [7]. 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 microelectronic 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

Important 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 can account for all these effects. In order to combine

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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 and then use this point response function in a three-dimensional convolution procedure developed earlier [3], [4] for the analytical simulation of ion implantation.

The point response function is a distribution function which would be obtained if the incoming ions hit only one specified point on the surface of the implantation target. If the entrance point of the ions is specified by the coordinates x_0 and y_0 on the surface of the sample, the point response distribution can be written as $P(x, y, z|x_0, y_0)$, where the x and y are the cartesian coordinates in the two lateral directions relative to the ion beam direction, and the coordinate z is aligned along the ion beam. Being a distribution function, the point response $P(x, y, z|x_0, y_0)$ is normalized to unity independently of the point of incidence (x_0, y_0):

$$\int\int\int P(x, y, z|x_0, y_0)\ dxdydz = 1. \quad (1)$$

If the point response function is known, the concentration distribution after an ion implantation step can be calculated as a convolution integral over the point response function:

$$C(x, y, z) = D \int\int P(x, y, z|x_0, y_0)\ dx_0 dy_0, \quad (2)$$

where D is the implantation dose and the integration region over the variables x_0 and y_0 covers the target surface exposed to the ion beam. The concentration distribution $C(x, y, z)$ is presented here in a beam aligned coordinate system.

The point response function to be used in the suggested combined method of simulation should be computed at a representative place of the simulated sample. A typical situation in microelectronic is that ions are implanted into silicon, and masks on top of the silicon define which parts of silicon are open for ion penetration and which are screened by the mask. Very sharp masks with almost vertical mask edges are typical for leading edge microelectronics. To minimize channeling and to prevent contamination, crystalline silicon is usually covered by a screening oxide of about 10 nm thickness. Since high accuracy of the simulation in silicon is required, a part of the device structure consisting of silicon and the screening oxide should be chosen for the simulation of the point response: When the point response is simulated in silicon covered by the screening oxide, the effects of the ion scattering in oxide on the channeling in silicon are accounted for. Furthermore, if a very small implantation window with a lateral size of about 1 nm is chosen for simulation of the point response, the spatial distribution of the implantation induced damage may be different from the damage distribution which is typical for the implantation using technological mask windows the size of which is often larger than 100 nm. Therefore, in order to correctly consider damage accumulation which results from a superposition of several damaged regions and has an influence on the implantation profiles, a sufficiently large implantation window with a lateral size comparable to the lateral range of the implanted ions has to be used for this simulation. To sum up, the following rules for the point response calculation can be suggested: 1) the implantation conditions (dose, energy and orientation of the ion beam relative to crystalline directions of silicon) are as specified in the implantation recipe; 2) the implantation window for the point response extraction has to be large enough to properly account for damage accumulation, e.g. larger than $3\Delta R_{pl}$, where ΔR_{pl} is the lateral straggling of the projected ranges; 3) a part of device structure consisting of crystalline silicon covered with screening oxide can be used as the implantation target for the point response calculation; 4) to extract the point response function, the results of the Monte-Carlo simulation have to be presented in a special coordinate system with the origin bound to the point of incidence of each simulated ion.

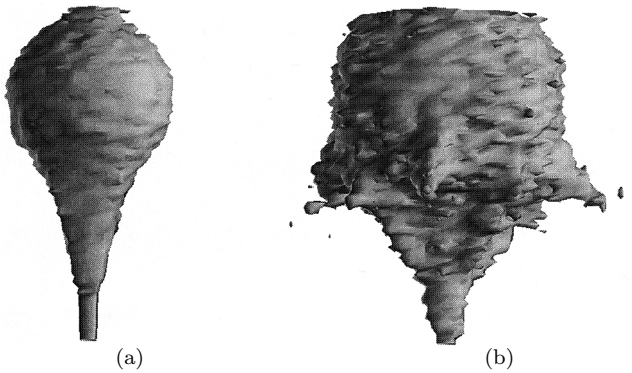

Fig. 1 Three-dimensional visualisation of the point response function for ion implantation of boron with an energy of 60 keV and a dose of $5{\cdot}10^{14}\,\mathrm{cm}^{-2}$ into silicon in crystalline direction <100> through a 10 nm oxide layer: (a) isoconcentration surface for a value of 1/100 of the function maximum, (b) isoconcentration surface for a value of 1/2500 of the function maximum.

The three-dimensional point response distribution function for implantation of 60 keV boron ions into crystalline silicon covered by a thin oxide layer is shown in Fig. 1. Normal incidence of the ion beam onto the sample is assumed. In the visualization the ion beam comes from the top of the figure. The point response has a relative simple cudgel-like shape for a concentration value equal to 1/100 of the maximum (Fig. 1(a)), however a more complicated shape for lower concentration values (Fig. 1(b)) is observed. The shape of the point response reflects the complicated channeling be-

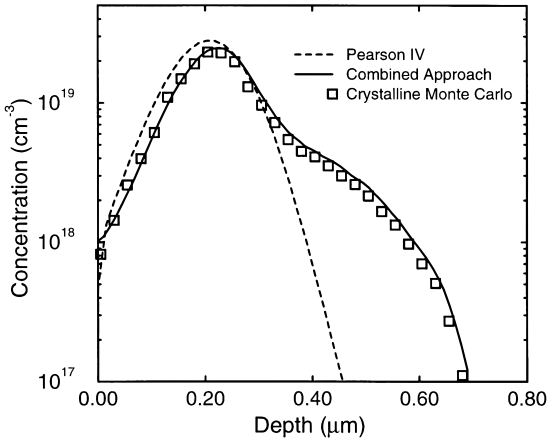

Fig. 2 Depth profiles of boron after ion implantation in <100> crystalline direction simulated with different methods.

havior of the boron ions in crystalline silicon. For a high concentration value, a main channeling direction along the <100> crystalline direction is seen. At lower concentrations, many channeling directions become effective.

To test the combined simulation approach we compared the depth profiles of boron after ion implantation with an energy of 60 keV and a dose of $5{\cdot}10^{14}\,\mathrm{cm}^{-2}$ simulated with the three methods: 1) using a conventional one-dimensional model based on the Pearson distribution of Type IV, 2) with a direct Monte-Carlo simulation and 3) using the suggested combined simulation method based on the usage of the numerical Monte-Carlo generated point response. The result is presented in Fig. 2. The conventional Pearson IV model uses model parameters for amorphous material and does not account for channeling. Therefore, the Pearson IV depth profile is shallower compared with that calculated with the Monte-Carlo method using the crystalline material model for silicon. Both the full Monte-Carlo method and the combined simulation method exhibit a typical channeling tail for larger depths. The combined simulation method agrees very well with the result of the full Monte-Carlo simulation. This means that the implemented convolution routine ensures sufficient accuracy of the convolution integration not only for regular analytical point response functions, but also for such complicated kernels as the point response function shown in Fig. 1.

3. Results of Three-Dimensional Simulations

To test the capabilities of the combined simulation method for the simulation of three-dimensional device structures, we used two types of three-dimensional samples for simulation of ion implantation. The first three-dimensional structure has sharp vertical edges and is similar to device structures created by anisotropic plasma etching, e.g. for shallow trench isolation in the

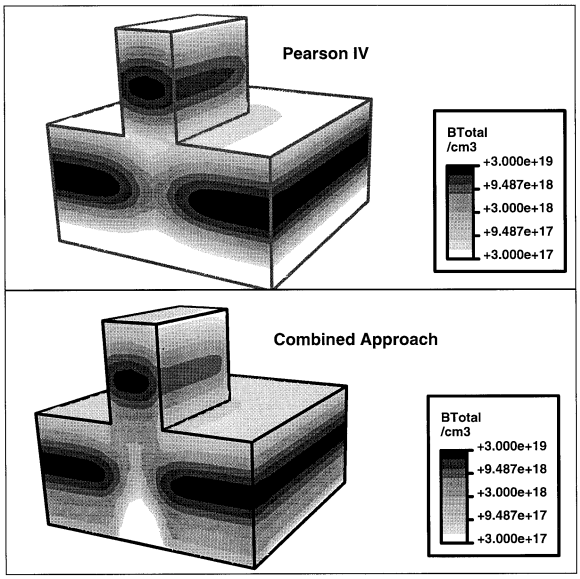

Fig. 3 Three-dimensional distributions of boron after ion implantation with an energy of 60 keV and a dose of $5{\cdot}10^{14}\,\mathrm{cm}^{-2}$ normal to the silicon surface in <100> crystalline direction simulated with the standard Pearson distribution and with the combined method using the Monte-Carlo generated point response.

CMOS technology. The lateral doping distribution in the samples with sharp mask edges is mainly determined by the shape of the point response. The second three-dimensional structure represents a silicon fragment close to a mask edge, and the mask edge is not vertical but tilted. In the case of tilted mask, as well as in the case of tilted ion implantation, the lateral shape of the resulting doping distribution is also influenced by the shape of the mask edges.

Figure 3 shows the simulation results for ion implantation of boron (60 keV, $5{\cdot}10^{14}\,\mathrm{cm}^{-2}$) into the sample with sharp edges. The target sample consists of two blocks of crystalline silicon with sizes of $1\times1\times0.5\,\mu\mathrm{m}^3$ and $0.24\times0.52\times0.4\,\mu\mathrm{m}^3$, respectively, and the upper surface of the silicon is covered with a 10 nm thick silicon oxide. The boron distribution resulting from the simulation using a conventional simulation model based on Pearson IV type depth distributions is depicted in the upper part of the figure, and the result of the simulation using the suggested combined simulation method is presented in the lower part of the figure. The implantation conditions of this implantation step are the same as in the one-dimensional simulation presented in Fig. 2, therefore the boron depth distributions at planar regions which are far enough from the mask edges are identical to those shown in Fig. 2. The simulation with the combined method exploits the point response function calculated using the physically based crystalline model and in this manner accounts for channeling. Therefore, a deeper ion penetration is seen in the prediction of the combined simulation.

For certain applications, e.g. for CMOS transistors

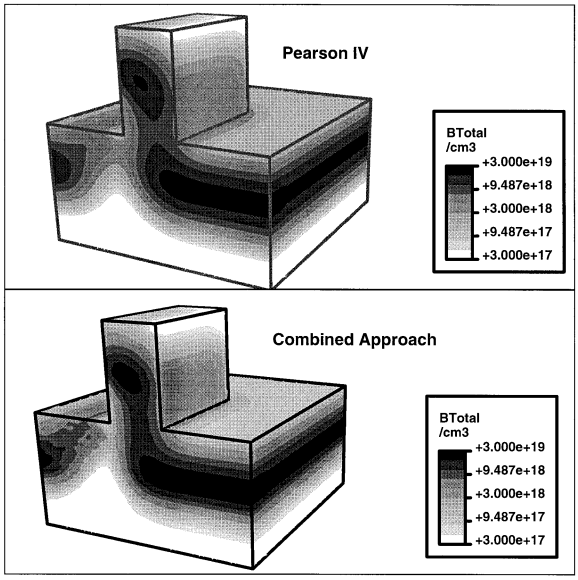

Fig. 4 Three-dimensional distributions of boron after tilted ion implantation with an energy of 60 keV and a dose of $5{\cdot}10^{14}\,\mathrm{cm}^{-2}$ (tilt 30°, rotation 22°) simulated with the standard Pearson distribution and with the combined method using the Monte-Carlo generated point response.

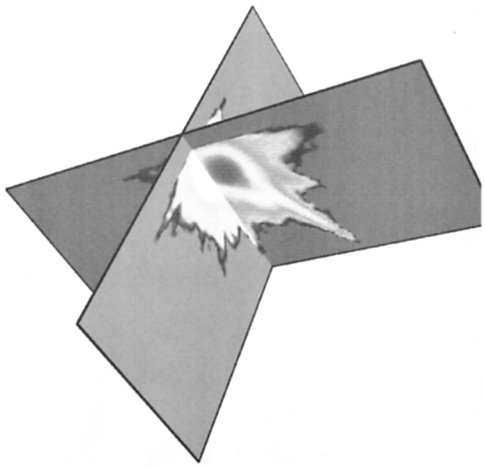

Fig. 5 Two cuts through a point response function resulting from an implantation of boron ions with an energy of 40 keV and a dose of $5{\cdot}10^{13}\,\mathrm{cm}^{-2}$ into silicon covered with 10 nm screening oxide. The ion beam was tilted by 7° in the plane which is the lateral cut plane in the figure.

with pocket type doping of the channel region, large angle tilted implantation is used. The large angle tilted implantation is more difficult for three-dimensional simulation, because of ion beam shadowing and multiple beam crossing of the sample surface. The inclusion of these effects in the convolution integral has been done based on the concept of the effective thickness [3] with standard models to account for different stopping in different layers [8], [9]. Figure 4 shows the doping distribution after a large angle tilted ion implantation of boron. The energy and dose of this implantation step are the same as used in the simulation shown in Fig. 3, but the ion beam was tilted by 30° and rotated by 22° from the front side plane (Fig. 4). To account for the different channeling for this incidence direction of the ion beam, a new point response has been calculated for this example using the Monte-Carlo method. Both, the analytical and the combined approach show an asymmetrical doping distribution formed due to the tilted implantation, but the shape of the distributions are slightly different. The difference between the two simulation methods is smaller in this case compared to the normal beam incidence because the channeling is suppressed for this implantation direction.

A very common implantation condition is the 7° tilted ion implantation often used to suppress channeling. We have simulated an implantation of 40 keV boron ions under 7° tilt angle into crystalline (100) silicon covered by 10 nm screening oxide. Figure 5 shows the point response distribution for this implantation. The relative boron concentration in a logarithmic scale from the maximum down to a value of 10^{-8} of the maximum is shown by different grey color densities on two cut planes. The ion beam was tilted in the lateral plane shown in Fig. 5. High concentration levels of the point response calculated have 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 along the <110> channeling direction. Also many other channeling directions are seen on this picture at lower concentrations. This means that the choice of 7° tilt does not completely suppress the channeling of boron and the shape of the point response has not a regular smooth shape like it is assumed in analytical models.

To compare the performance of the different simulation methods, we simulated ion implantation of boron with an energy of 40 keV and a dose of $5{\cdot}10^{13}\,\mathrm{cm}^{-2}$ into a silicon sample which is partly covered by a thick silicon dioxide mask with a 45° tilted edge. The area of the simulated silicon sample is $1 \times 1\,\mu\mathrm{m}^2$, the silicon substrate is covered with a 10 nm oxide, the mask thickness is $0.3\,\mu$m, and the onset of mask edge is located $0.375\,\mu$m from the edge of the silicon sample. Figure 6 shows the simulation results obtained with the analytical method (Fig. 6(a)) using a Pearson IV type point response function, with a full area Monte-Carlo simulation (Fig. 6(b)) and with the combined approach (Fig. 6(c)). The boron concentration is shown by different densities of the grey scale. The lightest grey density corresponds to an implant concentration of $1.5{\cdot}10^{16}\,\mathrm{cm}^{-3}$ and the darkest to $1.5{\cdot}10^{19}\,\mathrm{cm}^{-3}$. The analytical method underestimates the channeling effect while the doping profile calculated by the combined approach agrees very well with the Monte-Carlo simulation in the silicon region. Both, the full Monte-Carlo

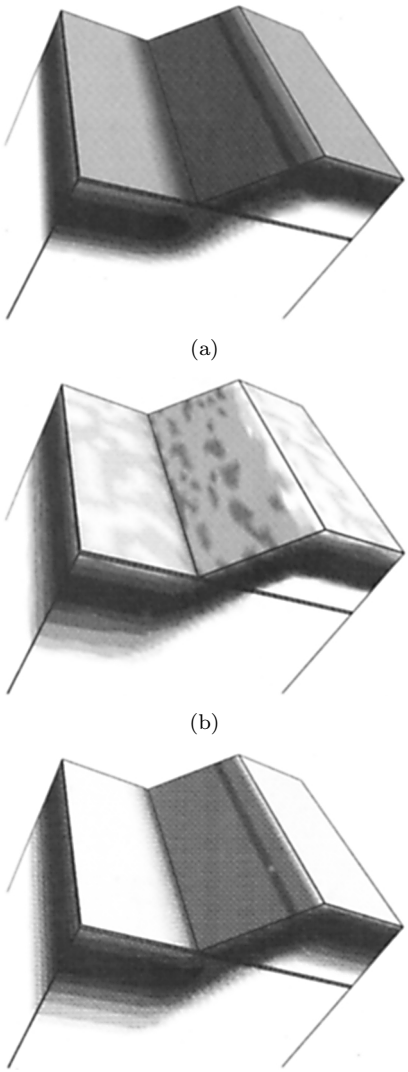

Fig. 6 Simulated boron distribution around an oxide mask edge resulting from an implantation of boron ions with an energy of 40 keV and a dose of $5{\cdot}10^{13}\,\mathrm{cm}^{-2}$. The ion beam was tilted by 7° in the plane parallel to the mask edge. The analytical method (a), the Monte-Carlo method (b) and the combined method (c) were used for the simulation, respectively.

and the combined simulation method result in similar doping distributions in silicon, in both methods the deeper penetration of the boron ions due to channeling is properly accounted for. A comparison of simulation results obtained by the analytical method, the combined method and the Monte-Carlo method demonstrates the increase in accuracy by using the combined method instead of a conventional analytical method.

The simulation times for the analytical method, the Monte-Carlo method and the combined simulation method are 6 min, 22 h 28 min, and 1 h 28 min, respectively. This means that for the example presented in Fig. 6 the simulation time of the combined method was by a factor 15 shorter than that for a complete Monte-Carlo simulation. A reduction of the computation time by using the suggested combined approach compared to a full area Monte-Carlo simulation can be achieved if the area of the structure for which the simulation should be performed is large compared to the area covered by the lateral extension of the point response function. The CPU time reduction factor can be estimated as the ratio of the full simulation domain to the area filled by the point response distribution and may result in a CPU time reduction by 10 to 1000, depending on the size of the simulation area and on implantation conditions.

To estimate the accuracy of the combined approach in comparison to a full Monte-Carlo simulation, we directly compared the results of these two simulation methods applied to the same implantation conditions and the same structure of the implantation target. Figures 7 and 8 show the iso-concentration lines in a vertical cut perpendicular to a mask edge. The implantation conditions in this comparison are the same as in the examples shown in Figs. 3 and 6, respectively. These two examples demonstrate a typical simulation accuracy for two limiting cases: a sharp mask edge and normal implantation direction (Fig. 7) and an oblique mask edge combined with a tilted ion implantation direction (Fig. 8).

The three-dimensional implantation target used for the simulation presented in Fig. 7 consisted of a silicon substrate covered by a 10 nm silicon oxide, and the right hand side of the sample was additionally covered by a polysilicon mask with a vertical edge. The thickness of the substrate silicon and of the implantation mask was taken as $0.9\,\mu$m to better observe the maximum ion penetration depth in silicon and to prevent a penetration of the ions through the mask. The full area of the implantation including masks amounted to $0.8\,\mu\mathrm{m}^2$. In Fig. 7, the part of the silicon located at lateral coordinate larger than $0.4\,\mu$m is covered by the mask, the left part of the sample at lateral coordinate less than $0.4\,\mu$m is only covered by 10 nm scattering oxide during implantation. To achieve a good statistical accuracy, $3{\cdot}10^6$ ion trajectories were used in the direct Monte-Carlo simulation and 10^5 ion trajectories for the simulation of the point response. In case of a sharp mask edge and normal implantation direction, the results of the combined approach reproduce the results of the direct Monte-Carlo simulation very well. The deviation between the two methods is of about 10 to maximum 30 nm. The lateral extension of the profile at the depth of the maximum of the boron distribution is reproduced with an accuracy of about 10 nm in the concentration range 10^{17} to $10^{19}\mathrm{cm}^{-3}$ using the combined method. This is a reasonable correspondence taking into consideration that the accuracy of the experimental methods to measure lateral distributions is not better than 10 nm and the typical cell size of the histograms used in the Monte-Carlo method is also of

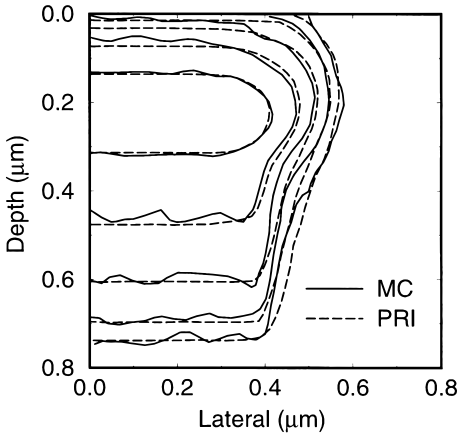

Fig. 7 Comparison of the boron distributions in silicon near a sharp mask edge simulated using direct Monte-Carlo method (MC) and the combined simulation approach based on the point response interface (PRI). The implantation conditions are as in the example presented in Fig. 3. Isoconcentration lines for 10^{17}, $3.2{\cdot}10^{17}$, 10^{18}, $3.2{\cdot}10^{18}$, and $10^{19}\,\mathrm{cm}^{-3}$ are shown.

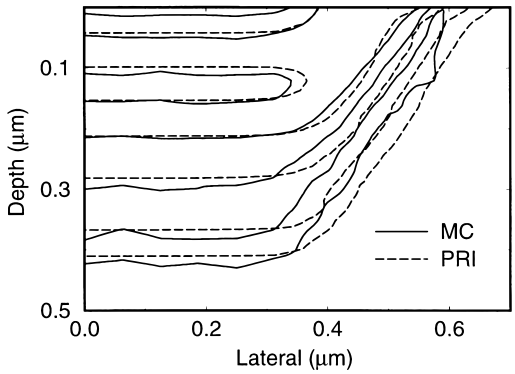

Fig. 8 Comparison of the boron distributions in silicon near a tilted mask edge simulated using direct Monte-Carlo method (MC) and the combined simulation approach based on the point response interface (PRI).The implantation conditions are as in the example presented in Fig. 6. Isoconcentration lines for $6.3{\cdot}10^{16}$, $2{\cdot}10^{17}$, $6.3{\cdot}10^{17}$, $2{\cdot}10^{18}$, and $6.3{\cdot}10^{18}\,\mathrm{cm}^{-3}$ are shown.

about 10 to 30 nm. Obviously, the convolution contained in the combined approach smooths the fluctuations associated in the Monte-Carlo simulations with both the statistics and the cell size used. A higher concentration of the boron implant in the Monte-Carlo simulation observed at the silicon surface can be explained by the contribution resulting from the ions scattered from the edge of the mask. This contribution is only partially accounted for in the combined approach.

The iso-concentration lines of boron distributions shown in Fig. 8 were directly extracted from the results of the simulations shown in Figs. 6(b) and 6(c). Boron distributions in silicon simulated using the full Monte-Carlo method and the combined method based on the point response interface are shown. The mask edge is located at $0.3\,\mu$m of the lateral coordinate shown in Fig. 8. The right hand side of the sample is covered by the mask, and the shape of this oblique mask is depicted in Fig. 6. A somewhat less good overall accuracy compared to the case of a vertical mask edge is observed. The deviation between the results obtained with the two methods amounts 10 to 35 nm. The largest deviations are observed under the edge of the oblique mask. There are two main reasons for this deviation. First, the combined method in this initial implementation seems to overestimate the penetration of the ions through the oxide mask, but this can be easily improved by a calibration of the parameters of the multi-layer models [8], [9] specially for the use in the combined method. Second, the Monte-Carlo method has a tendency to underestimate the penetration through thick masks because of the low probability of such events. When estimating the accuracy of the simulation of ion implantation, we have to keep in mind that an average distance to the next neighbor for implanted ions at a concentration of $10^{17}\,\mathrm{cm}^{-3}$ is of about 20 nm and fluctuations of the distance to the next neighbor up to 40 nm are probable. Therefore, even if the same number of ion trajectories as in real implantation is used in the Monte-Carlo simulation, fluctuations of the isoline positions due to statistical effects are existent and they are comparable with the accuracy of the combined approach in the present simulations.

4. Conclusion

Using a point response function extracted from Monte-Carlo simulation and the CPU time efficient algorithm for three-dimensional convolution developed earlier, a point response based interface between the Monte-Carlo and analytical simulation methods was established. The simulation results of the suggested combined approach are almost as accurate as a full area Monte-Carlo simulation but require significantly less computation time.

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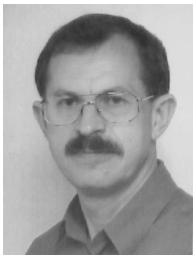

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Klaus Tietzel was born in Roth near Nuremberg, Germany, in 1966. He received his *Dipl.-Phys.* degree from the *Friedrich-Alexander-Universität Erlangen-Nürnberg* in 1993. Since 1994 he has been with the *Fraunhofer-Institut für Integrierte Schaltungen* where he prepared his doctoral thesis devoted to three-dimensional simulation of ion implantation and recently received his *Doctor* degree. Dr. Tietzel contributed to the European projects *PROMPT* and *PROMPT II* through development of software for three-dimensional simulation of ion implantation in microelectronics.

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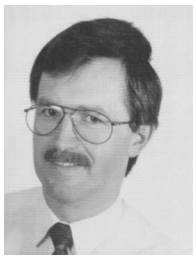

Jürgen Lorenz was born in Stockelsdorf, Germany, in 1957. He studied physics and mathematics from 1976 to 1983 at the *Universität Hamburg* and at the *Technische Universität München* where he completed his *Dipl.-Math.* and *Dipl.-Phys.* degrees in 1982 and 1984, respectively. In 1983, he joined the *Fraunhofer-Institut für Festkörpertechnologie* in Munich, working in the field of process modeling and simulation. In 1985, he moved to the newly founded *Fraunhofer-Arbeitsgruppe für Integrierte Schaltungen* where he has since then been in charge of the modeling and simulation department. His present research areas are the development of process models and simulation software for ion implantation, dopant diffusion, oxidation and layer deposition steps. Jürgen Lorenz has authored or co-authored more than 80 papers in the fields of process modeling and simulation, and has been responsible as coordinator for various research projects in these fields, among others the ESPRIT projects PROMPT and PROMPT II on the development of a novel three-dimensional process simulation system.

Heiner Ryssel received his *Dipl.-Ing.* degree in electrical engineering in 1967, and his *Dr. Ing.* degree in 1973, both from the *Technische Hochschule*, Munich, Germany. From 1968 to 1972, he was with the *Institut für Technische Elektronik*, working on GaAs epitaxy and ion implantation. In 1973, he joined the *Institut für Integrierte Schaltungen* where he worked on ion implantation in Si, Ge, and III-V compounds. In 1974, he joined the *Institut für Festkoerpertechnologie*, Munich, where he worked in the area of semiconductor device development and basic implantation studies. Since 1985 he has been professor of electrical engineering at the *Universität Erlangen-Nürnberg*, and director of the *Fraunhofer-Institut für Integrierte Schaltungen* in Erlangen. His main research topics are process modeling, semiconductor processing equipment, and advanced process development.

Siegfried Selberherr was born in Klosterneuburg, Austria, in 1955. He received the degree of Dipl.-Ing. in Control Theory and Industrial Electronics from the Technical University of Vienna in 1978. Since that time he joined the *Institut für Allgemeine Elektrotechnik und Elektronik*, previously called the *Institut für Physikalische Elektronik*, at the Technical University of Vienna. He finished his doctoral thesis on "Two Dimensional MOS Transistor Modeling" in 1981. Dr. Selberherr has been holding the *venia docendi* on computer-aided design since 1984. He is the head of the *Institut für Mikroelektronik* since 1988 and since 1999 he is dean of the *Fakultät für Elektrotechnik*. His current topics are modeling and simulation of problems for microelectronics engineering. He authored and coauthored more than 300 publications in journals and conference proceedings. Furthermore, he wrote a book *Analysis and Simulation of Semiconductor Devices*. Dr. Selberherr is member of the *Association for Computing Machinery* (1979), the *Society of Industrial and Applied Mathematics* (1980) and the *The Institute of Electrical and Electronics Engineers* (M'79, SM'84, F'93). Dr. Selberherr is editor of the Springer-Verlag book series *Computational Microelectronics*.