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Three-dimensional Process Simulation for Advanced Silicon Semiconductor Devices

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Abstract — *The fabrication of advanced semiconductor devices makes heavy demands on the simulation. The main directions for ongoing research are on the one hand the extension of the simulation tools to three spatial dimensions and on the other hand the development of more sophisticated physical models.*

1 Introduction

The simulation of technological processes for the fabrication of semiconductor devices has been world-wide established as an essential tool for both the improvement of existing and the development of new fabrication processes. Obtaining as input the type of material, the geometry, and the individual process steps the simulation has to provide a sufficiently accurate description of the resulting device. This description consists of the topography and of the properties of the material ("doping profile") at the surface as well as in the interior of the device. Although this contribution deals with the simulation of technological processes only, it should be stated that for practical applications the process simulation can not be regarded in an isolated manner from device simulation: just the coupling of both yields an efficient tool for design and optimization of semiconductor devices where the interface is built by the doping profile.

The dramatic progress in semiconductor technology with respect to shrinking dimensions of single devices and increasing die sizes of integrated circuits leads to extremely complex connections between the parameters within a single process step as well as between succeeding process steps. While some years ago two-dimensional — in some cases even one-dimensional — models were sufficient, nowadays, due to the miniaturization, a variety of phenomena can be taken into account only by three-dimensional process simulation. Thus, the unique trend for research and development goes towards program packages which account for all three spatial dimensions. Nevertheless, owing to the enormous amount of computing resources they will not supersede the two-dimensional simulators in the near future for standard applications.

The most important process steps for the manufacture of advanced silicon devices, e.g., lithography, etching, deposition, ion implantation, diffusion, and oxidation, are included

in state-of-the-art process simulators. Owing to lack of space this contribution will focus only on the simulation of ion implantation and topography.

2 Ion Implantation

Ion implantation is currently the most important technique for introducing dopants into semiconductors. As modern annealing methods (e.g., Rapid Thermal Annealing) do not alter the implanted profile very much, the determination of the initial implantation profile has become a very important task. Thus the simulation of ion implantation gained in significance tremendously. For the simulation three main techniques can be used: The analytical description of the doping profile [1], [2], the solution of the Boltzmann transport equation [3], [4] or the Monte Carlo method [5], [6], [7].

The analytical method usually has the benefit of minor demands on CPU-time consumption. One-dimensional profiles can be modeled accurately by the analytical description of profiles. Already for two-dimensional computations problems arise, because of the lack of an underlying physical base for multi-dimensional extensions of this technique. The limitations can be seen on examples with tilted implantations or with abrupt changes of the simulation geometry as demonstrated in Fig. 1 where the results of the simulation of an implantation of boron with a tilt angle of 0° and an energy of 100 keV into an idealized trench are shown. The thin lines represent the concentration of boron related

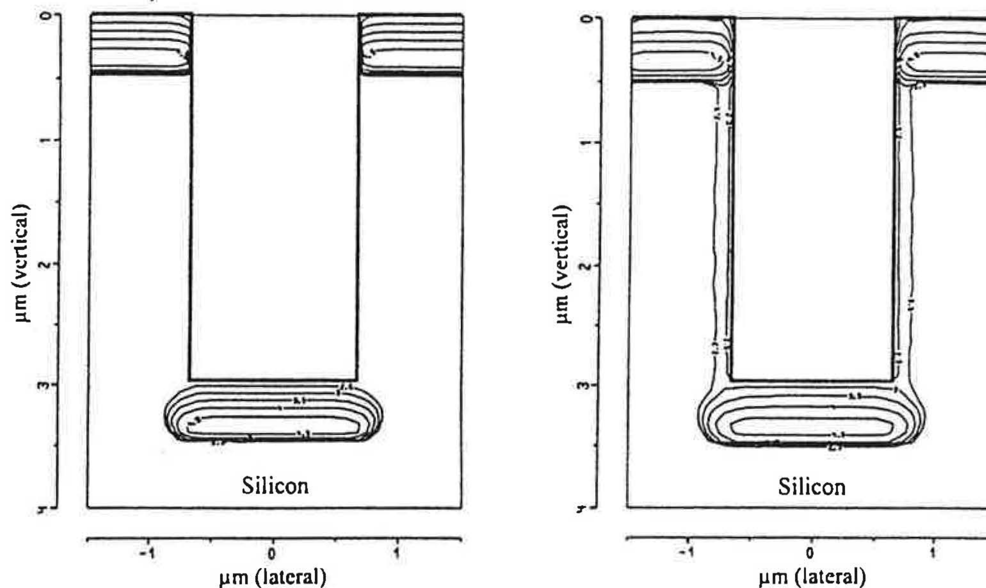

Figure 1: Trench simulation with analytic (left) and Monte Carlo method (right)

to the dose on a logarithmic scale in the range of 2.5–4.5 with an increment of 0.5. The analytic method (left part of Fig. 1) yields no concentration at the side walls of the trench because the distribution function nearly vanishes at a certain depth. However, the Monte Carlo method (right part of Fig. 1) shows a significant boron density there which results from particles entering the side wall after they have been reflected by the opposite one.

The solution of the Boltzmann transport equation is very efficient and accurately possible for one-dimensional applications [3]. For two-dimensional simulations the CPU-time and memory requirements increase significantly. Nevertheless, this method can be still advantageous compared to the two-dimensional Monte Carlo methods, when demands on accuracy are not too high. For three-dimensional simulations this method is despite today's computer power not applicable.

For the above listed reasons the Monte Carlo method is the choice for three-dimensional problems, although some special considerations are necessary to reduce the otherwise tremendous CPU-time consumption: up to some millions of ion paths (*"trajectories"*) must be calculated in order to obtain enough statistical information in regions with low but not negligible concentrations. Fig. 2 shows one typical trajectory schematically: after

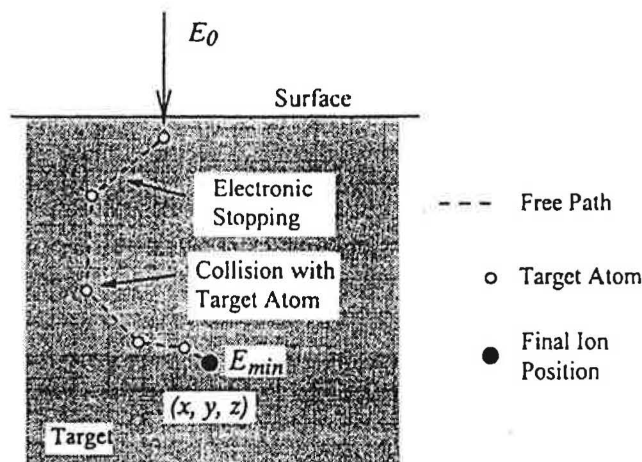

Figure 2: Trajectory of an implanted ion

entering the substrate material the ion successively collides with target atoms where it looses some portion of energy and is scattered randomly. Between two collisions the ion energy is decreased by the so-called electronic stopping power which results from the interaction of the electrons of the ion and the target atoms. The physical models for the scattering mechanism as well as the electronic stopping shall not be discussed here but some techniques to accelerate the simulation: First a superposition method is used to decrease the number of collision events to be evaluated [8], second an octree has been introduced for the discretization of the geometry to simplify the point location problem [9], and third a trajectory split method dramatically reduces the required computational effort even for the simulation of ion implantation into crystalline structures [5].

2.1 Superposition Method

This acceleration method is based on the idea to use the information obtained by one calculated trajectory more than once. At the beginning a model trajectory is computed for each material in the simulation area and then this model trajectory is copied several times to the whole simulation window. By this technique from a few thousand model trajectories about a million physical trajectories can be derived. In this manner the number

of collision event evaluations and therefore the CPU-time consumption are decreased. But the computation time required for the necessary geometry checks for the point location remains the same. It should be noted that this method can be applied to amorphous targets only, because ion implantation into crystalline substrates implies a transient aspect: Owing to the ion bombardment the crystal structure is locally damaged and an accumulation of these point-defects leads to an amorphous behavior of the material.

2.2 Octree Discretization

The octree method comes from graphical image processing [10]. For this method a cube (the root cube) is constructed first that contains the whole simulation area. This cube is then subdivided into eight sub cubes as can be seen in the left part of Fig. 3. This procedure is recursively continued for each sub cube until either the desired accuracy of the discretization is reached or no more intersections of this cube with the polygons defining the target geometry exist. For every leaf-cube the material which it contains is

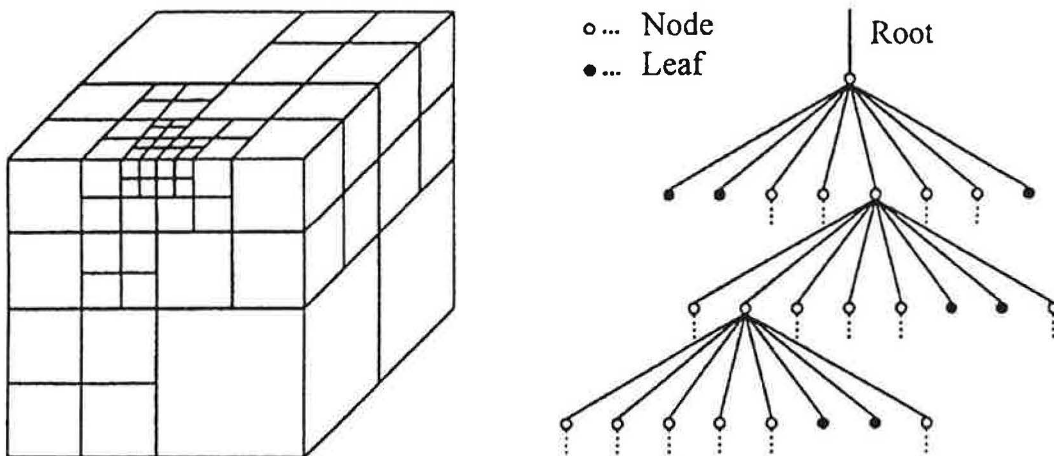

Figure 3: Octree discretization (left) and data structure (right)

determined; one leaf can only contain one material. Later then, for the point location simple inequality comparisons can be used. The octree is stored as a tree in the memory as can be seen in Fig. 3. This method speeds up the simulation tremendously. The computation time required for one trajectory is nearly independent of the regarded number of spatial dimensions.

2.3 Trajectory Split Method

Since the majority of ion trajectories ends at the most probable penetration depth, the statistical noise of regions with a dopant concentration several orders of magnitudes smaller than the maximum cannot be tolerated — the solution for that problem is to increase the total number of calculated ion paths. The fundamental idea of this simulation approach is now to locally increase the number of calculated trajectories in areas with large

statistical uncertainty by splitting up the trajectories depending on the ratio of the current local concentration C_{loc} and the current global maximum density of dopants C_{max}: if C_{loc}/C_{max} at the trajectory point under consideration falls short of a certain limit this point becomes a split point from which two trajectory branches will start unless the ion moves from lower to higher local concentration. Therefore this approach is a self-adaptive algorithm, because more split points are defined in those areas only with unsatisfying statistical accuracy. The peripheral regions of the dopant concentration are represented by a much higher number of ion trajectories and the statistical noise is reduced.

In contrast to the superposition method which is restricted to amorphous materials, trajectory splitting can also be applied to the simulation of ion implantation into crystalline targets and especially for that purpose this method is of essential relevance. Despite the considerable decrease of computing effort obtained by the trajectory split method (about a factor of $\frac{1}{5}$) a further reduction of the turn around time of three-dimensional simulations is necessary. From the actual point of view, the only promising way seems to be a migration to highly parallel algorithms.

3 Topography

Topography simulation deals with the basic processes of pattern definition and pattern transfer which ultimately change the shape of the wafer surface. The numerical algorithms for surface movement play a key role in those simulators and lead to major differences in accuracy, robustness, and efficiency of the simulation tools.

Basically there are two types of algorithms used for modeling three-dimensional topography processes. Volume removal methods [11] divide the material being etched into a large array of rectangular prismatic cells. Each cell is characterized as etched, unetched or partially etched. During etching cells are removed one by one according to the local etch rate and the number of cell faces exposed to the etching medium. These methods which are successfully used in three-dimensional lithography simulation [12] can easily handle arbitrary geometries, but unfortunately they suffer from inherent inaccuracy, because they favor certain etch directions.

Surface advancement methods on the other hand represent the surface of the material being etched by using a mesh of points which are connected by line segments to form triangular or rectangular facets. Depending on the implementation either the mesh points or the facets are moved according to the local etch rates. A mesh management is necessary to maintain the mesh as it moves in time. In general, surface advancement algorithms — the most prominent one is the well known string-algorithm [13] — offer highly accurate results, though with potential topological instabilities such as erroneous surface loops which result from a growing or etching surface intersecting with itself. The surface loops must be removed before they become too complex which is a rather complicated task in three-dimensional simulation [14].

A recently developed and very efficient general approach [15] for the surface movement is based on fundamental morphological operations used in image and signal processing [16] and allows accurate simulation of arbitrary three-dimensional structures without loop formation. The simulation geometry is basically considered as a two-valued image (material or vacuum), and an array of square or cubic cells is used where each cell is characterized as etched or unetched. As illustrated in Fig. 4, a material identifier is defined for each cell,

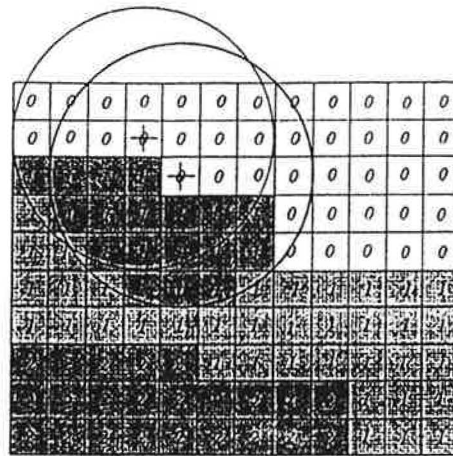

Figure 4: Material representation and structuring element

therefore material boundaries need not be explicitly represented. The surface or etching boundary consists of unetched cells that are in contact with fully etched cells. Cells on the surface are exposed to the etching medium or to the deposition source, and etching or deposition proceeds on this surface. A linked surface cell list stores dynamically etch or deposition rates of exposed cells.

To advance the etch front spatial filter operations based on the erosion or dilation operation [16] are performed along the surface boundary. During an etching process, all cells whose centers lie within a filter are etched away, while cells outside stay unchanged. Usually, for isotropic three-dimensional simulations filters are spheres (see Fig. 4 and left

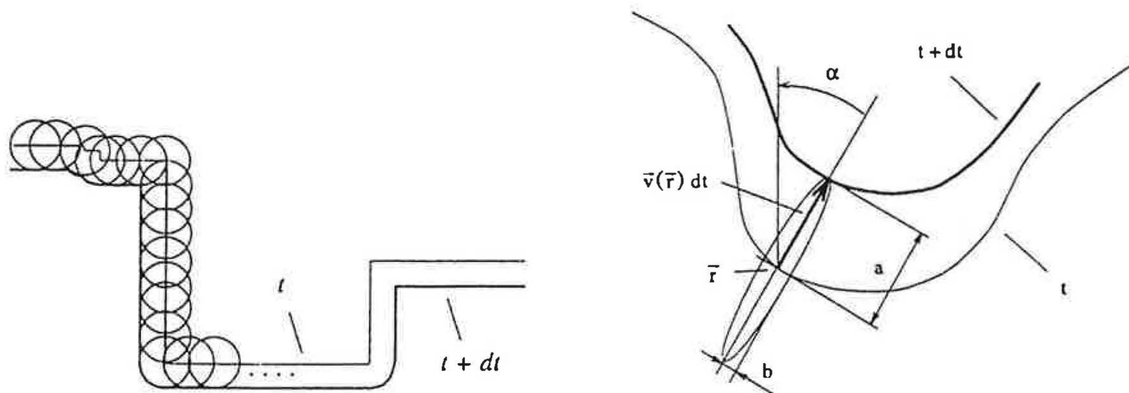

Figure 5: Schematic representation of an isotropic etching process (left) and structuring element for anisotropic surface advancement (right)

part of Fig. 5), and for anisotropic movement of surface points filters are ellipsoids (right part of Fig. 5), although there is no restriction on the filter shape. The spatial dimension of an applied filter determines how far a surface point moves. The main axes of an ellipsoid are given by the local etch or deposition rates multiplied by the time step. After each time

step the exposed boundary has to be determined by scanning all the cells in the material. Material cells are surface cells if at least one cell side is in contact with an already etched cell. The exposed sides of the detected surface cells describe the etch or deposition front at a certain time step.

When the surface passes from one material to another, filter operations must be performed by using composite filters. The important question is how the surface evolves at the boundary, since interfaces lead to an abrupt change in etch rates. Therefore, filter operations are performed selectively on a given material. That means, filter operations on cells of a given material will only remove cells of the same material. If a filter extends over a material boundary it demands an additional filter operation performed selectively to the second material. The etch rate for this second filter operation is calculated regarding the etch rates on both side of the interface and depending on how far the filter reaches into the other material.

Fig. 6 shows the cross-section of an etched contact hole as a result of three-dimensional simulation. The simulated process consists of two etching steps: The first one is a wet chemical process with an etching rate of 0.5 nm/s and a duration of 1000 s. One can clearly see that the lateral material removal below the quadratic mask is as wide as into the depth owing to this isotropic etching step. The second step is directional with a chemical etching rate of 0.65 nm/s and a duration of 500 s which transfers the mask geometry nearly without lateral material removal. Note that the top plane of the simulation area does not represent the surface of the mask in order to be able to simulate the succeeding metallization process without changing the simulation geometry.

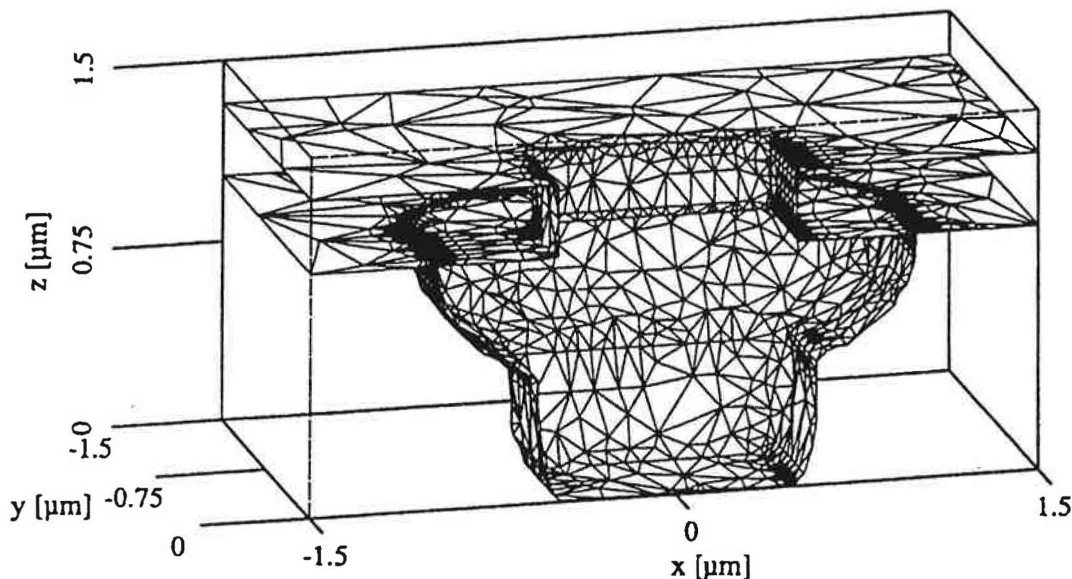

Figure 6: Etching of a contact hole

The general surface advancement method yields a highly efficient and very stable topography simulation tool. Care has to be taken about the discretization: The structuring element must contain enough cells in order to avoid unrecoverable positioning errors of the moving surface.

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