THREE DIMENSIONAL MONTE CARLO SIMULATION OF ION IMPLANTATION WITH OCTREE BASED POINT LOCATION

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To increase the amount of devices on a constant wafer area a change from the common two-dimensional (2D) structures to a three-dimensional (3D) layout is suggested for modern semiconductor devices. Therefore modern process simulators must be capable of modeling these 3D structures. A simulation tool using the Monte Carlo method for ion implantation with the ability of modeling realistic, complex 3D structures has been developed. The main problem which is the geometry check in the 3D space, is discussed.

In recent times, many speed up techniques have been developed to improve the performance of multidimensional Monte Carlo simulation tools for ion implantation to make them applicable for every day usage [1], [2]. Usually these tools perform quasi-3D simulations meaning that even when they really compute ion trajectories in a 3D space, for the geometry checks it is assumed that the target is infinite at least in the third direction. An approach for the simulation of selected 3D geometries is presented in [3]. In this paper, implants into differently shaped trenches are presented.

To make simulations at all possible in a 3D space, a superposition method [4] is used to allow for the simulation of a large number of ions in order to obtain good statistics in reasonable computation times. For this method the implantation window is first divided into subwindows. Then a model trajectory is precomputed, assuming an infinite target. This trajectory is then copied into every subwindow, so that out of one physically computed trajectory several effective trajectories can be derived. If the particle crosses a boundary between different regions of the simulation area, the pre-computed trajectory is interchanged with another one for the new material. This method minimizes only the computation of the collision events for one trajectory group, whereas the geometric checks have to performed for each effective trajectory. Consequently, most of the simulation time is consumed to detect whether the particles cross a boundary in the 3D case.

Since the general geometries which are accepted as input can not be limited to convex or otherwise restricted shapes the determination of intersections of geometry boundaries with the trajectory is very complex and time consuming. Therefore a so-called "**octree**" was introduced for the representation of the geometric data. By use of the octree the geometry is discretized into cubes. Every cube is recursively subdivided into eight subcubes until either the desired accuracy of the discretization is reached – which is measured by the sidelength of the cube – or no intersection of this cube with the polygones of the geometry exists (see Figure 1). Once the octree has been created, for the simulation of ion trajectories simple comparisons can be used instead of very complicated and numerically sensitive computations of intersections. To determine the location of an ion, just a simple test of the coordinate against the related coordinates of the sidewalls of the cube is required, because the cube is aligned with the coordinate axes. This leads to a drastic decrease in computation time compared to other methods. Beside the reduction of computing time, the octree also simplifies the coupling of this module with 3D topography simulators which are based on cellular methods. To clarify the concept of an octree, a triangle which is discretized by a quadtree – this is the 2D equivalent to an octree – is shown in Figure 2.

As an example the simulation of an arsenic implantation step (As with 100keV, no tilt angle) into a structure derived from topographic simulations is presented. The geometry which was generated by a new tool for the simulation of etching and deposition, can be seen in Figure 3. In Figures 4 – 6 the results are shown. Due to the symmetric conditions uniform profiles are obtained. The computation for this example took less than one hour of computation time on an HP 9000/730.

REFERENCES

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[4] G. Hobler and S. Selberherr, *Monte Carlo Simulation of Ion Implantation into Two- and Three-Dimensional Structures*, IEEE Trans. CAD, Vol. 8, No. 5, pp. 450-459, Mai 1989.

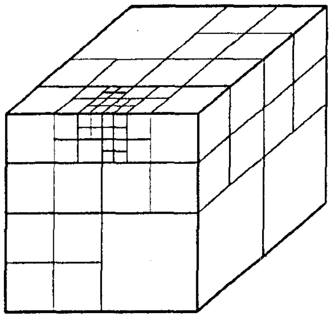

Figure 1: Discretization using an octree

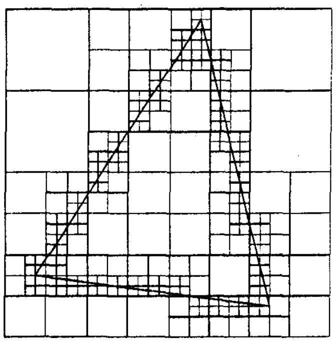

Figure 2: Discretization of a triangle

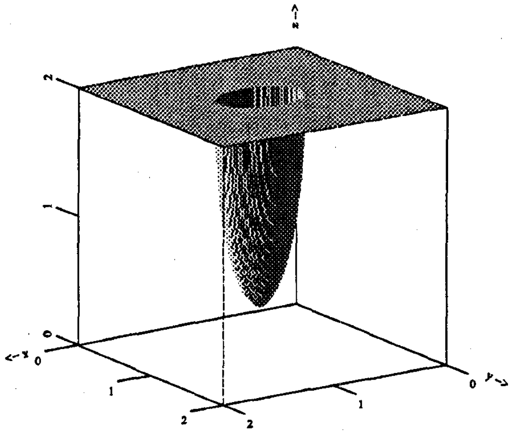

Figure 3: Geometry derived from topography simulation

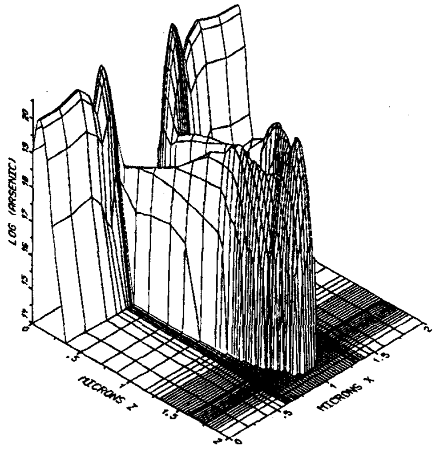

Figure 4: Intersection for constant y coordinate (y = 1 μm)

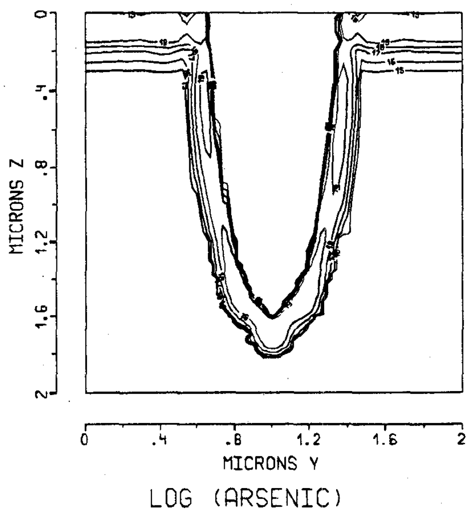

Figure 5: Intersection for constant x coordinate (x = 1 μm)

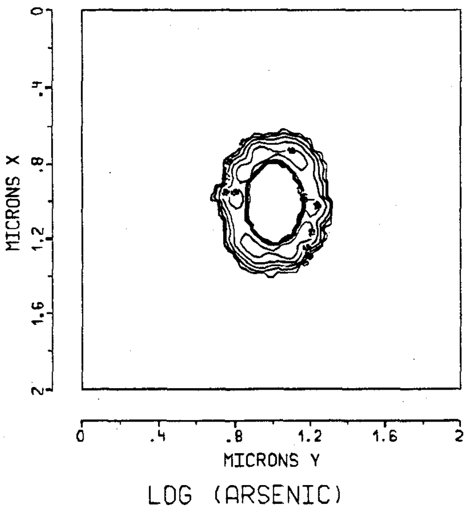

Figure 6: Intersection for constant z coordinate (z = 1.15 μm)