# ADAPTIVE TESSELLATION FOR THE THREE-DIMENSIONAL SIMULATION OF DOPING PROFILES

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## ABSTRACT

We present a new process simulation module which is capable of solving the coupled nonlinear partial differential equations of diffusion problems in three space dimensions. An adaptive gridding method has been developed in order to handle geometries consisting of multiple material regions of arbitrary shape.

## INTRODUCTION

Fast and accurate simulation of three-dimensional redistribution processes requires both automatic grid adaptation and fast equation solvers. The computational grid determines the size and the condition of the linear equation system and therefore, it is mostly responsible for simulation efficiency. In diffusion processes, the dopand profiles are changing their shape with time and thus, automatic grid adaptation is required.

## ADAPTATION STRATEGY

For resolving the boundaries and interfaces of the computational domain a coarse initial tessellation is used. The elements of this tessellation are refined by means of a recursive element decomposition method until the desired accuracy is reached.
Due to an object oriented design our algorithm works on mixed element grids and is not restricted to any kind of special element shapes. Two types of elements are currently implemented: the tetrahedron and the octahedron, both using linear shape functions.
On refinement we divide a tetrahedron into four small tetrahedra and one octahedron. The small tetrahedra are located at the parents corners, and the remaining part has octahedral shape (Fig. 1). An octahedron is split into six small octahedra at each corner and the eight remaining tetrahedra between them (Fig. 2).
The chosen refinement rules ensure that the child elements inherit the parents shape even during multiple refinement steps. This feature preserves a good condition of the nonlinear equation systems.

## SIMULATION STRATEGY

For the practical use of the refinement method we estimate the discretization error by means of a gradient smoothing method [1] which is used throughout the whole simulation.
At beginning of the simulation, the initial grid is adapted to the initial impurity distribution. After each timestep elements with a large discretization error get refined whereas elements with a small

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discretization error are replaced by their parent elements. This algorithm ensures that a fine mesh is located only where it is really needed.
In order to solve the system of nonlinear equations we use a damped Newton iteration scheme, which is based on a highly efficient linear solver [2]. Further we implemented a time step control according the discretization error. Therefore, our simulator allows to compute results for realistic three-dimensional applications within acceptable demands on computational resources.

## EXAMPLE OF A BORON DIFFUSION STEP

To demonstrate the benefits of the adaptive gridding algorithm, we computed a diffusion step for a Boron channel-implant in a conventional LOCOS-structure at 1000°C and an annealing time of 30min. Figure **??** shows the coarse initial tessellation of the simulation region where the field oxide is on top of the silicon bulk. The channel implant has been computed by a Monte-Carlo ion implantation simulation module [3] with an enery of 20keV and a dose of 1e14cm$^{-2}$. The initial grid has been adapted to the initial profile for a discretization error limit of 1% relative to the total implanted dosis. The grid for the silicon region with the distribution is shown in Figure **??** and consists of 9534 nodes and 19259 elements.
As the diffusion advances the steep gradients are smoothed and therefore, the grid was reduced continuously by the automatic adaptation algorithm. Thus, the final grid at the end of the simulation consists of only 4282 nodes and 8836 elements (Fig. **??**).
For the needed 34 timesteps the program consumed a CPU-time of 41 minutes at an HP9000-735 workstation and used approximately 23MB of memory, which shows, that fully three-dimensional diffusion simulation with a controlled discretization error is feasible.

## ACKNOWLEDGEMENT

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[3] W. Bohmayr and S. Selberherr. Trajectory Split Method for Monte Carlo Simulation of Ion Implantation Demonstrated by Three-Dimensional Poly-Buffered LOCOS Field Oxide Corners. VLSI-TSA 95, Taipei.

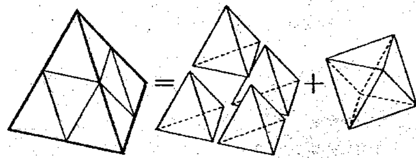


Figure 1: Tessellation for a tetrahedron

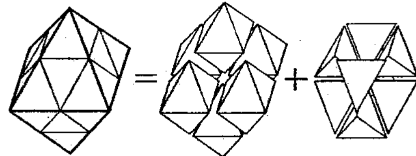


Figure 2: Tessellation for an octahedron

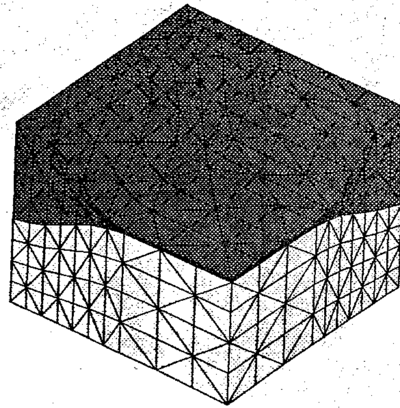
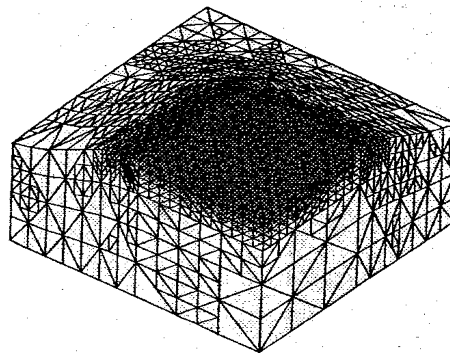


Figure 3: Corner of the LOCOS structure



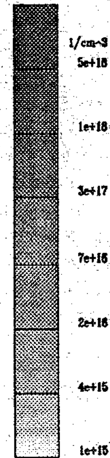
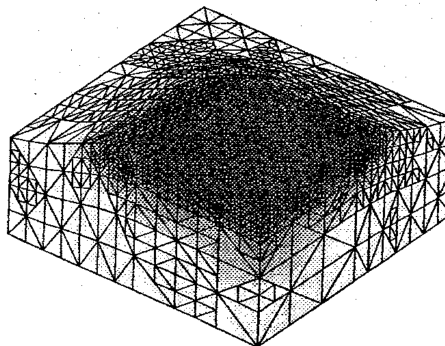



Figure 4: The implanted Boron profile in the Silicon region



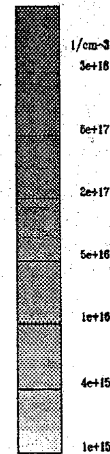



Figure 5: Boron profile after 30min. annealing at 1000°C