Efficient 3D Mesh Adaptation in Diffusion Simulation

Tao Chen, Daniel W. Yergeau, Robert W. Dutton
CISX 305, Integrated Circuits Laboratory, Dept. of Electrical Engineering,
Stanford University, Stanford, CA 94305

Abstract

Diffusion simulation is an important part in today's TCAD research. While many works have been done on 2D mesh adaptations in diffusion simulation [1] [2] [3], 3D mesh adapation remains a challenging area due to the excessive amount of grid points most mesh generation algorithms produce. In this paper, we apply a generalized octree grid generation algorithm for mesh adaptation. It has the advantage of reducing the number of nodes necessary for accurate simulations.

A generalized octree mesh generation algorithm [5] enables mesh refinement and derefinement in different directions at various regions. A vector level control function is computed and indicates the directions for which the refinement will be performed. In a contour based refinement scheme, the level control function indicates the directions as the gradient, while in an error estimator based scheme, it indicates the direction where the error will be maximally reduced. Every octant can be refined in either one, two or three dimensions. After the tree is generated, detailed tetrahedralization algorithms are implemented to match the complex geometry and ensure mesh comformalty. Then after each simulation step, the vector level control function is re-calculated according to the new gradient or error, and the mesh is adapted to reflect the changing areas of simulation significance. With the tree structure, interpolation error is also greatly reduced since the meshes before and after the adaptation share many common nodes.

A generic finite element dial-an-operator PDE solver [4] is used to implement the diffusion simulator. An operator is a dimensionally independent discretized representation of a term in a PDE and it generates residual vector and tangent matrix to be used by a nonlinear solver. Grouping operators into equations and systems produces the coupled systems of equations to be simulated. Flexible description of physical models is enabled by changing the equations and operators.

Both the mesh server and the diffusion solver reside in a TCAD framework controlled by Tcl scripts. A typical session will involve first generating a mesh according to an initial implantation profile. The diffusion solver then performs a time step of transient simulation with the mesh and the result is fed back to the mesh server. A new mesh is generated and used for another time step of simulation. The process is repeated until the total diffusion time is reached. Fig. 1 shows a boron diffusion with segregation in a hole structure, and Fig. 2 shows a boron diffusion in a MOSFET. We see that new nodes are added efficiently to reflect the changing position of the junctions and old nodes are removed when they no longer have simulation significance.

References

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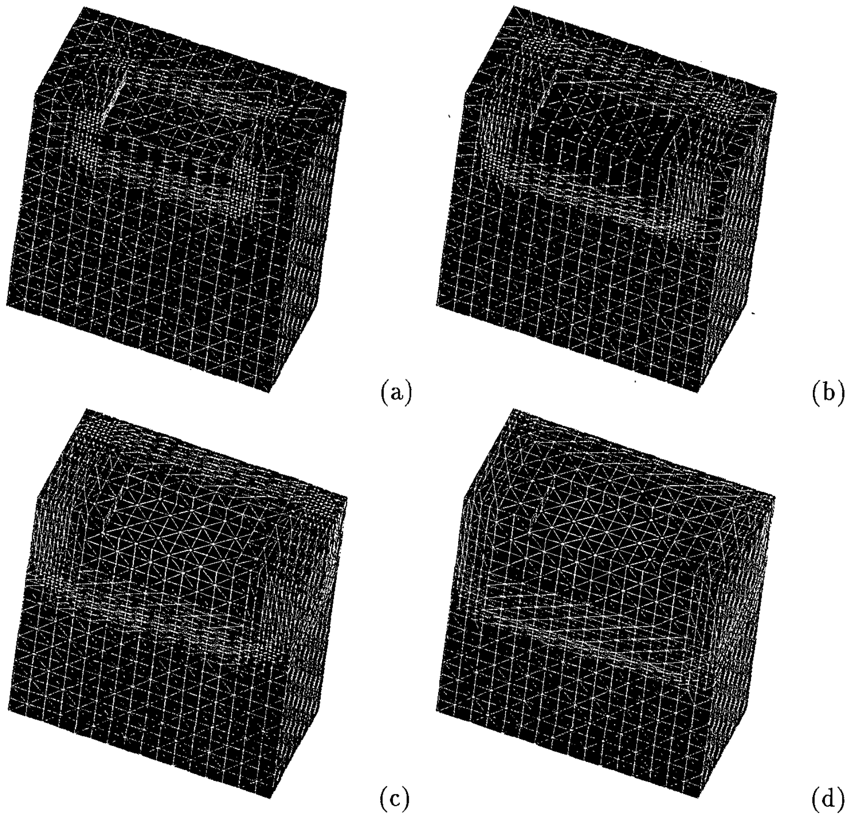

Figure 1: Boron diffusion in a hole structure at 1100 °C. The four meshes are a) initial mesh (t = 0 seconds), b) adapted mesh at t = 240 sec, c) adapted mesh at t = 480 sec, d) adapted mesh at t = 720 sec, respectively.

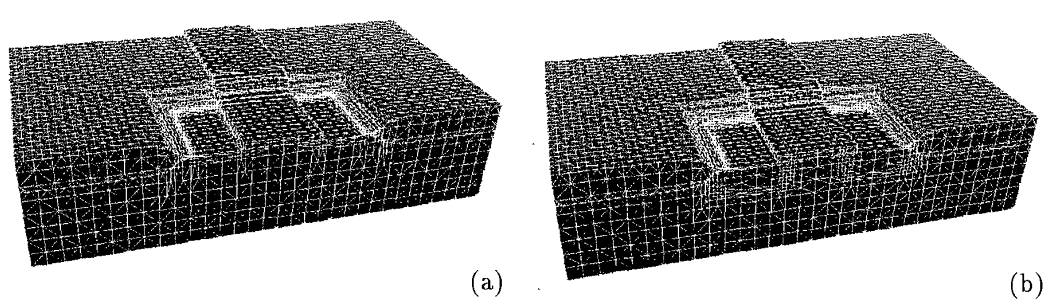

Figure 2: Boron diffusion in a MOSFET at 1100 °C. a) initial mesh. b) final mesh at t = 900 sec.