2-D Adaptive Simulation of Dopant Implantation and Diffusion

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Abstract

This paper describes the techniques for adaptive grid generation for dopant implantation and diffusion in process simulation.

1. Introduction

Mesh generation and adaption for solving dopant diffusion in process simulation is a difficult task, complicated by both the moving boundaries of oxide growth and the time dependence of the solutions. For both computational and ease of use reasons, automatic mesh generation and discretization error control is desirable. This paper describes an approach based on local error estimates [1] to refine the mesh. The results presented in this paper extend our previous work [2] to two-dimensional problems. The implementation of this approach is done in a process simulator FLorida Object-Oriented Process Simulator (FLOOPS.)

2. Nodal Error Estimation

In the one dimensional part of this work, the Bank-Weiser [3] error estimator appears to be the most promising. For process simulation, the discretization error is proportional to the curvature. This is easy to compute and use. The error is used to implement the grid adaption algorithm in two dimensions and also applied to mesh refinement in self-adaptive grid generation procedure. In the benchmark, the parameter for refinement is varied from 1 to 0.1 and the coarsening parameter is one tenth of the refinement parameter. The result shows that the dopant concentration errors and profile junction depth errors are bounded and controlled by the refinement within 8% and 6% respectively when compared to solution computed on a fixed grid spacing of 10 Å. The total dose interpolation errors, critical for adaptive simulation, are within 0.2%.

3. Grid Quality Issue on Local Refinement

A smoothing technique is required to improve the grid quality after local refinement. Two approaches can be used to solve this problem, one is by Laplacian smoothing, the other is by solving an optimization problem with regard to triangulation quality[4]. The global smoothing procedure moves every grid node in the mesh to a new location, and requires the interpolation of

solutions onto the new position. Two approaches for dopant interpolation have been investigated. The first is based on the dose conservation law. The second approach for solution interpolation utilizes the upwinding concept. The primarily result of utilizing smoothing and interpolation technique on the local refinement was presented for single dopant simulation[5]. In Figs 1-2, a test is carried out by simulation of a SideWAll-Masked Isolation (SWAMI) structure with a channel stop implant by Boron dose of $5x10^{15}$ cm^{-2}, 30 keV. The final structure is grown for 60 minutes in 1000 ^{o}C anneal under a wet oxygen ambient. The resulting structure demonstrates the capability of mesh adaption for dopant diffusion with moving boundaries. During the 60 minutes diffusion, mesh smoothing is carried out in each time step. In Fig. 1, the computed junction depth by dose normalization technique is shallower than the ones by upwinding technique. This is due the restriction of grid movement imposed upon dose normalization approach to ensure the validity of local dose conservation law. In general, the usage of the upwinding technique for interpolation is preferred since it allows faster computation. The two smoothing techniques are about the same though the Laplacian average approach shows slightly better improvement of final grid quality. The most promising is the smoothing by triangle quality optimization and the interpolation by upwinding. The smoothing is also applied to the oxide layer during oxidation. This improves the grid quality along the silicon/ oxide interfaces.

4. Applications

In order to exercise the robustness of this adaptive algorithm, the front-end to fabricate a CMOS inverter by a twin-well process is simulated with FLOOPS and the resulting grid for the isolation is shown in Fig. 3. This shows the grid adaption capability beyond the silicon layer. It allows the treatment of grid refinement or smoothing in multiple materials. The multi-layer and multi-dopant aspects therefore can be illustrated through this realistic example.

5. Conclusion

A new approach for adaptive simulation for dopant in implantation and diffusion is presented. It's suitable for multi-layer and multi-dopant in 2-D and can be extended for 3-D process simulation.

References

[1] M. Bieterman, I. Babuska, "The finite element method for parabolic equations, I. A posteriori error estimation," *Num. Math.*, vol. 40, p.339,1982.

[2] C. C. Lin, M. E. Law, and R. E. Lowther, "Automatic Grid Refinement and Higher Order Flux Discretizations of Diffusion Modeling," *IEEE Trans. Computer-Aided Design*, vol. CAD-4, No. 12, p. 436, Aug. 1993.

[3] R. E. Bank, A. Weiser, "Some a posteriori error estimators for elliptic partial differential equations," *Math. Computation*, vol. 44, p.283, 1985.

[4] C. C. Lin, M. E. Law, "Mesh Adaption and Flux Discretizations for Dopant Diffusion Modeling," *NUPAD V Proceeding*, p. 151, Honolulu, June,1995.

[5] R. E. Bank, "Moving Mesh," *NSF/SEMATECH Workshop on Gridding in VLSI TCAD*, section V, Mar. 1994.

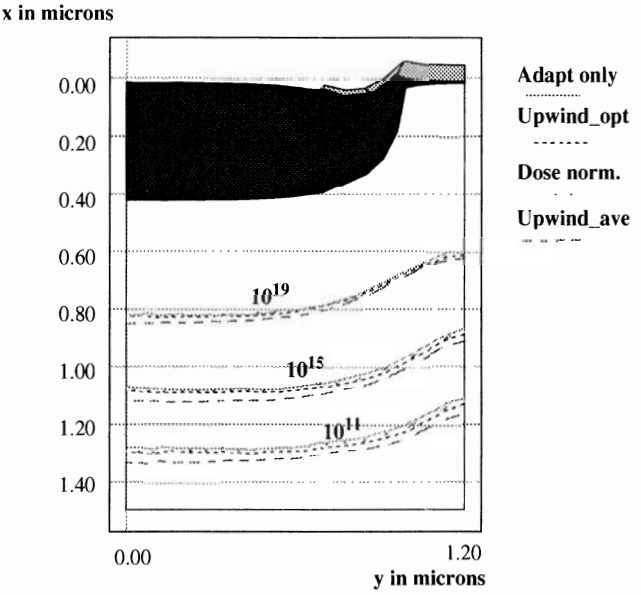

Fig. 1 The contours of dopant solution after the growth of SWAMI.

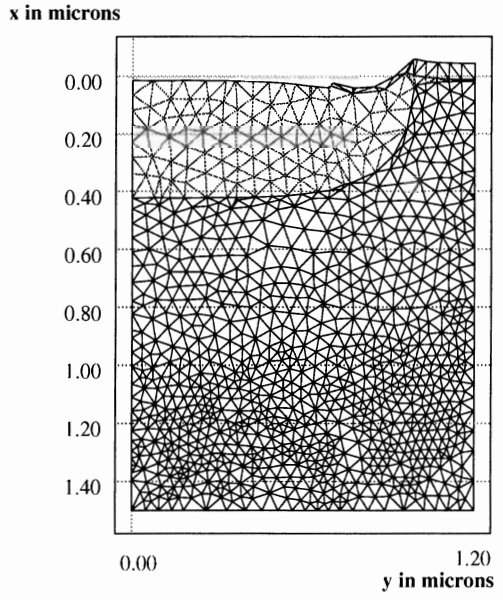

Fig. 2 The resulting smoothed mesh after the growth of SWAMI.

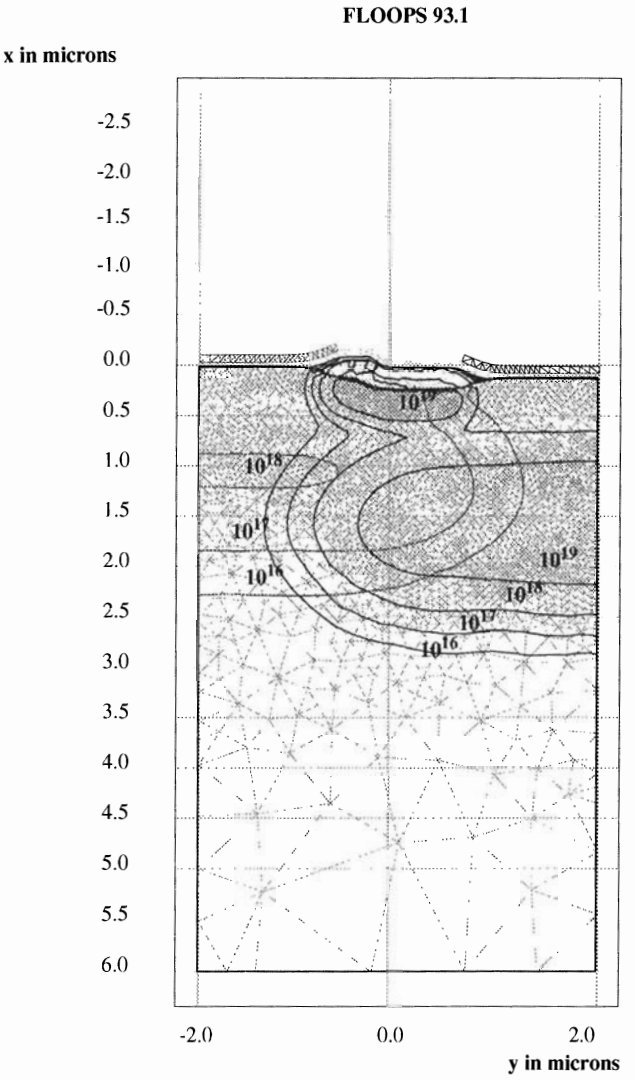

Fig. 3 The wells and isolation structure for a twin-well CMOS process.