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Process Simulation for Nonplanar Structures with the Multigrid Solver LiSS

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Abstract

This paper presents the application of LiSS, the 2D multigrid solver for parabolic and elliptic differential equations developed by the GMD, to the simulation of diffusion processes in complex nonplanar structures. A domain-splitting method is presented. The behaviour of different multigrid cycles applied to rectangular and curvilinear grids of a trench structure is investigated.

1. Introduction

Multigrid methods have been applied successfully to planar diffusion [1] and oxidation problems [2]. In our approach we used the general purpose multigrid solver LiSS [3], implemented a discretization scheme for the diffusion equations and applied it to several complex structures.

The underlying equations for the N_{EQ} diffusing species are

$$\frac{\partial C_i}{\partial t} + \mathrm{div}\left(\sum_{j=1}^{N_{EQ}} a_{i,j} \cdot \mathrm{grad} C_j + b_i \cdot C_i \mathrm{grad}\psi\right) + \gamma_i = 0 \qquad i = 1, \ldots, N_{EQ} \quad (1)$$

with assumed local charge neutrality. The applied diffusion models are fully compatible with those of PROMIS [4]. The discretization of the equations has been done using a finite volume approach on a nine point stencil, the resulting set of nonlinear equations is solved by a Newton iteration scheme.

In this approach the whole domain is divided into blocks. For each block a boundary-fitted logically rectangular grid is generated with a biharmonic generator also using a fast multigrid algorithm. This technique provides a high geometric flexibility. Thus it enables the solution of a wide range of problems and reduces numerical problems due to distortions.

2. Multigrid Strategy

Multigrid algorithms have been developed to overcome two disadvantages of iterative solvers such as SOR, first the so called h-dependent convergence behaviour which results in slower convergence for finer grids and second the initially good reduction of both residual and error norms which becomes worse with an increasing number of iterations.

A multigrid solver mainly consists of four parts: the smoothing, the restriction, the injection method, and finally the cycle type. The *smoother* makes the error a smooth function over the whole domain. Relaxation methods are used for this purpose, because they damp high-frequent residual-"modes" very efficiently. By means of the *restriction* method the residuals are transferred from one level (or grid) to the next coarser level. The *prolongation* method defines how to transfer the residuals from one level to the next finer level. Finally the *cycle type* defines how many smoothing

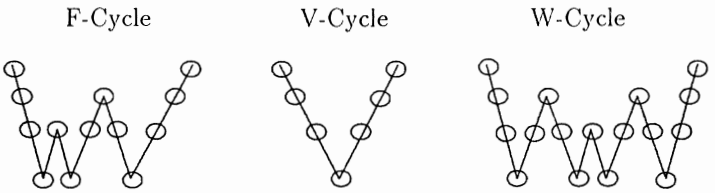


Figure 1: Multigrid Cycle-Types

steps should be performed on each level and the sequence of the different levels as shown in Fig. 1. For example a $V(\nu_{down}, \nu_{up})$ cycle performs ν_{down} smoothing steps before restricting to the next coarser level and ν_{up} smoothing steps after prolongation from the coarser level. The proper choice of these components has great impact to the efficiency of the algorithm.

3. A Trench Problem

A practical application is a "simple" trench as shown in Fig. 2 (boron background doping, arsenic source/drain implant with a 7^o tilt angle). In this case the domain is

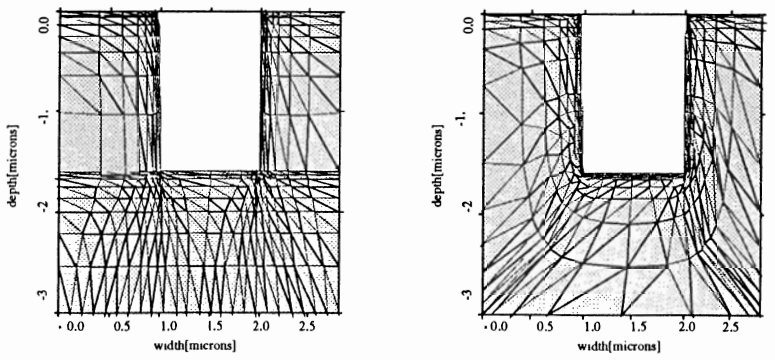
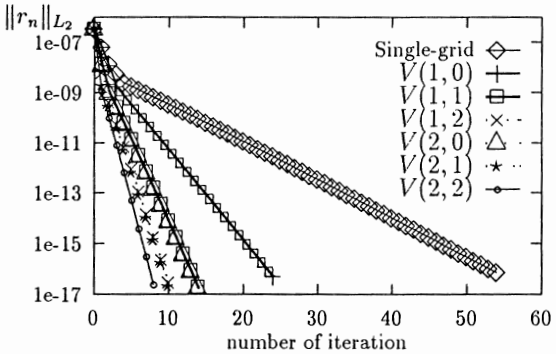


Figure 2: The trench geometry with a block structured grid (a) and a conventional grid (b) (The triangles are an effect of the visualization of non-orthoproduct grids)

split into three nearly rectangular blocks where a grid is generated separately for each of them. In regions near to the boundaries, where high dopant gradients occur, the grids have been refined. From Fig. 2a the advantage of block–splitting, mentioned in section 1 (distortion), becomes obvious. This becomes even more important when treating more complicated structures such as undercuts.

The multigrid method used for this example consists of the following components. As *smoother* a Gauss–Seidel relaxation has been applied. *Restriction* was done by "full weighting", which uses the local average of the residuals on the finer level. The *prolongation* is a simple linear interpolation. The cycle is of V-type with different parameters ν_{down} and ν_{up}, respectively. The table of Fig. 3 shows the residual history, the runtimes and the convergence rates of various combinations of cycle parameters. Note that for higher values of $\nu_{down} + \nu_{up}$ the convergence is faster, but it should be noted that the computational effort rises, too. As these results show, the multigrid-cylce takes about half the computation time of a single-grid cycle. The experiments showed that a $V(2,1)$-Cycle provides excellent results for a wide range of problems. For a small number of cycles the convergence rate of the single-grid cycle is in the same



Cycle	Time/s	$\frac{\|r_n\|_{L_2}}{\|r_{n-1}\|_{L_2}}$
SG	2115	0.702
V(1,0)	1299	0.437
V(1,1)	1336	0.222
V(1,2)	1242	0.126
V(2,0)	1237	0.223
V(2,1)	1234	0.125
V(2,2)	1266	0.079

Figure 3: Residual reduction of a single-grid solver, multigrid solver with various cycles, their runtimes and their convergence rates

range as the convergence rate of a multigrid cycle (see Fig. 3 for the first 3 iterations). After a few iterations the high frequent residual–modes have been smoothed and the remaining residual is dominated by low–frequent modes. For these low-frequent modes single-grid methods are very inefficient as Fig. 3 shows. In contrast to the single-grid method the multigrid-method does not show this effect. Although the computational effort of a multigrid cylce is a multiple (almost twice as much) of the effort a single-grid method (depending on the cycle-parameters ν_{down},ν_{up}), the multigrid method is significantly faster because of the constant and fast convergence for all cycles.

These tests have been performed with both types of grids shown in Fig. 2. The runtimes for the same number of unknowns are approximately the same for both grid types. Against the expectations the curvilinear grid from Fig. 2b did not lead to convergence or accuracy problems. However, the advantage (with respect to computation time) of the blockstructured grid is obvious since the blocks can be handled in parallel only exchanging information at their common boundaries.

The physical results of the computation are presented in Fig. 4. The diffusion was performed at 1000°C for 20 minutes. The results for the one-dimensional part on

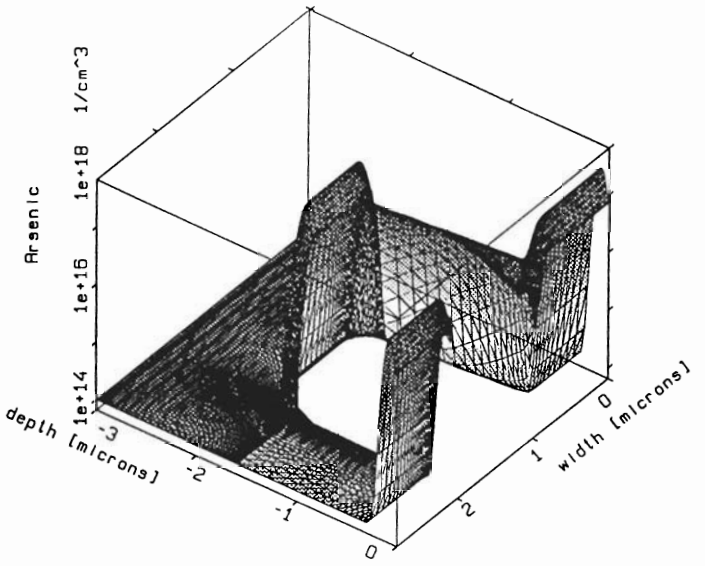


Figure 4: Final dopant distribution in the trench

the right side of the trench have been compared with a PROMIS simulation giving excellent agreement. The differences between the solutions were caused only by the different time step sizes, this means by the time discretization error.

4. Conclusion

This work has been an investigation about the suitability of the general purpose solver LiSS for the simulation of diffusion problems. The results obtained fit well with theorectical predictions. Convergence properties of the multigrid methods are very good, assuming that suitable multigrid components are in use.

Acknowledgement

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References

[1] Mijalković, S.; *An adaptive multigrid algorithm for simulation of diffusion processes in semiconductor device fabrication*, Electrosoft, Vol. 1, No. 4, pp. 277-290 (1990)

[2] Joppich, W.; *Mehrgitterverfahren für Diffusionsprobleme der Prozeßsimulation*, PhD-Thesis Universität Bonn (in german)

[3] Lonsdale, G.; Stüben K.; *The LiSS Package*, Gesellschaft für Mathematik und Datenverarbeitung m.b.H

[4] Hobler, G.; Pichler, P.; Wimmer, K.; *Promis 1.5*, Technical University Vienna, Institute for Microelectronics