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Simulation of Thermal Oxidation and Diffusion Processes by Parallel PDE Solver L$_i$SS

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In this paper a rigorous approach to simulate thermal oxidation and diffusion phenomena is presented. Because the numerical problems will increase in future, especially when looking towards three-dimensional process simulation, special emphasis is laid upon a parallel approach which additionally uses an optimal order solution method. The multigrid method is known to be an efficient tool for flow problems and for diffusion problems [2]. The different processes which are to be considered, oxide flow and diffusion of dopant, are usually described by completely different partial differential equations (PDEs) on the respective domain. Therefore the whole problem belongs to the class of what we call multiphysics problem. The different subtasks are defined on different domains which are coupled via conditions at the Si-SiO_2-interface. This multistructure situation combined with the multiphysics character of the underlying application requires new tools both for the development of models and for the investigation of parallelization aspects, which are indispensable for the next generation of simulation methods. Based on an environment for the parallel solution of elliptic and parabolic PDEs, L$_i$SS [1], such a tool was developed. The finite volume method is used to discretize the problems on time dependent domains, leading to moving grids in each of the subdomains. The coupling strategy offers a wide range of coupling intensity. It can be selected to couple the problems only after each time step, within the multigrid solution process after each multigrid cycle, after pre- or post-relaxation and between other algorithmic components.

Although L$_i$SS is not a process simulator, it is known, that this tool can be used efficiently for the simulation of diffusion processes [3]. For this work the implantation was done by PROMIS from the Technical University of Vienna. Initial profiles have been created with Pearson IV descriptions for the bird's beak geometry and by Monte Carlo methods for the trench geometry. The oxide flow is modeled as stress-dependent viscous flow with the stress-dependent diffusion coefficient and reaction rate of the oxidant. The impurity diffusion is described by vacancy diffusion coefficient model, taking oxidation enhancement into account.

References

[1] H. Ritzdorf, A. Schüller, B. Steckel and K. Stueben, "L$_i$SS – An environment for the parallel multigrid solution of partial differential equations on general 2D domains" *Parallel Computing*, vol. 20, pp. 1559-1570, 1994.

[2] W. Joppich and S. Mijalković, *Multigrid methods for process simulation.* Series *Computational Microelectronics*, edited by S. Selberherr, Wien: Springer–Verlag, 1993.

[3] R. Strasser, G. Nanz and W. Joppich, "Process simulation for nonplanar structures with the multigrid solver L$_i$SS ," in *Simulation of semiconductor devices and processes - vol.5*, S. Selberherr, H. Stippel, and E. Strasser, Eds., pp. 417–420, Wien: Springer-Verlag, Sep. 1993.

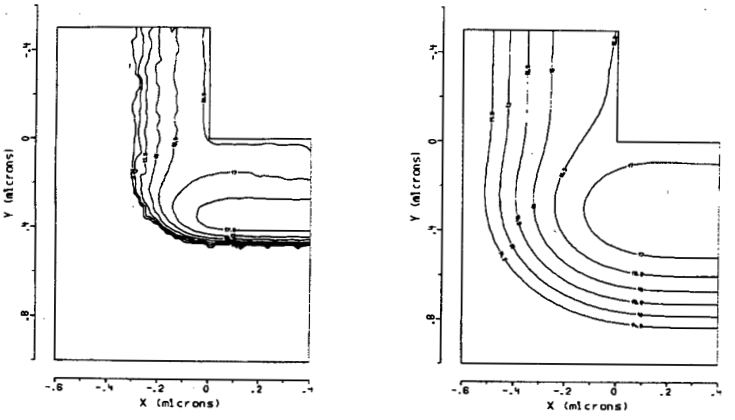

Figure 1: Diffusion on a trench, initial state generated by MC method with PROMIS, TU Vienna and result obtained by L$_i$SS after 70 minutes

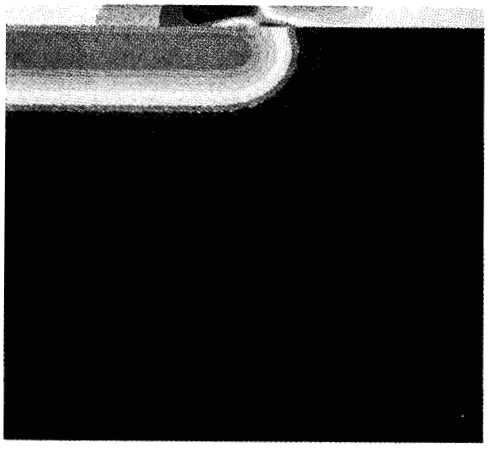

Figure 2: Initial geometry, pressure in SiO_2, Boron profile (logarithmic) in Si

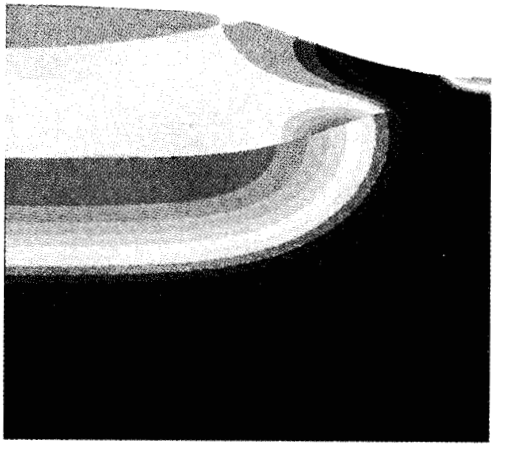

Figure 3: Geometry after 30 minutes, pressure in SiO_2, Boron profile (logarithmic) in Si

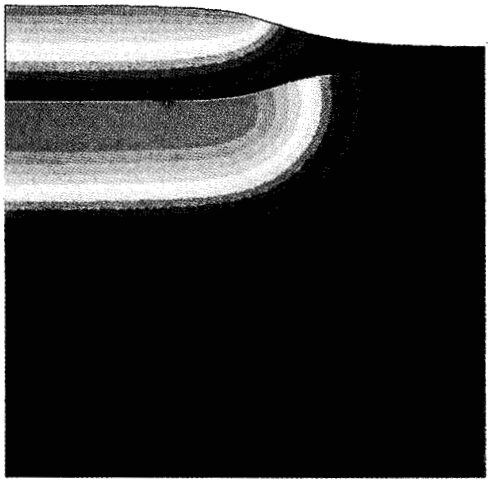

Figure 4: Concentration of oxigen in SiO_2, Boron profile (logarithmic) in Si

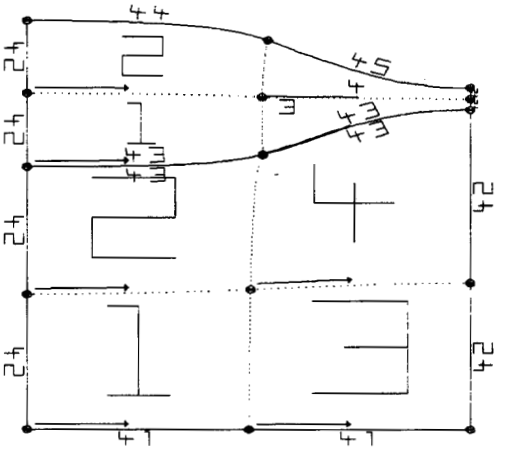

Figure 5: Final geometry, underlying block-structure for the parallel computation