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Chapter 7. Summary and Conclusions

The work presented in this thesis describes the design and development of a computational modeling and simulation environment to study Plasma Enhanced Chemical Vapor Deposition (PECVD). We call this environment the 'Virtual Reactor'. The PECVD processes are notoriously complicated with many intricate multi-scale, multi-physics and multi-chemical aspects. The Virtual Reactor should support a better understanding of these processes and assist in designing and optimizing real experiments. The challenge was to find the right level of detail and abstraction of all the related processes that still gives us an adequate, reliable and computationally efficient view into the PECVD processes.

Chapters 2 and 3 describe the physics and chemistry as well as the numerical models needed to study PECVD with flow in 1, 2 and 3 dimensions and with a 1-dimensional plasma model. In our simulations, we studied the parameters considered to be important for either adjusting or assessing reactor performance, such as the flow rate, reactor volume, silane dilution, discharge gap and substrate separation in plasma configuration. Comparison with experimental data demonstrated the ability of the model to predict the film growth rate and concentrations of individual components with reasonable accuracy. It was shown that the widely used technique of diluting silane with molecular hydrogen increases the growth rate and reduces production of higher silanes, thus making this technology more economical and ecologically clean. Numerical simulation indicated that the effective decomposition of silylyl outside the discharge zone reduces its contribution to film growth as the substrate is moved away from the discharge. The analytical expressions obtained for silyl and silylyl fluxes and for the profile of atomic hydrogen closely approximate the results of our numerical simulations. Real-life reactors are often not symmetrical, therefore the influence of reactor geometry on the actual gas flow needed further study. For that we developed a 2D and 3D numerical gas flow simulation, to study in detail the influence of reactor configuration on the flow field and on the deposition homogeneity. We observed that in some process conditions both 3D and 2D simulations predict that radial distribution of main parameters (e.g. species concentrations) along the wafer is almost ideally symmetrical with the axis of symmetry in the center of the wafer. This indicates that the homogeneity of these parameters near the wafer was mainly defined by the diffusive transport and not the convection. In some other cases, however (with a high flow rate) the symmetry was broken, which means that a full 3D simulation is essential to correctly predict the homogeneity of the deposition process. The Virtual Reactor allowed us to study also the film degradation processes and to find the featuring trends in system response to the variation of physical and chemical parameters. We were able to indicate the mechanisms responsible for the layer composition at the finishing stage of the film production cycle.

We did however observe a mismatch between the experimental and simulated distribution of the film thickness along the substrate. Additional numerical experiments indicated that the correct (experimental) shape can be recovered by adjusting the electron density distribution rather than gas flow parameters and substrate temperature distribution.

We therefore conclude that a 2D discharge model is needed. This model we implemented in Chapter 4. The simulation results in this Chapter show a qualitatively good agreement of the simulated results with the experimental data in the film distribution shape and the observed thickness variation. We also obtained a good correlation of measured film properties with the simulated ion and radical fluxes towards the substrate. In addition we studied the influence of pressure, temperature and plasma discharge parameters (power and frequency) on the PECVD processes in a wide range of parameters. These results clearly indicated that the Virtual Reactor is capable of predicting trends in the most relevant film growth parameters and can be used for studying, predicting and optimizing the PECVD technology. In addition it was shown that even small changes in the inlet and outlet position can significantly affect the uniformity and composition of the growing film. We conclude from this that the deposition characteristics are sensitive to the *complete* experimental parameter space.

After having established reliable numerical models for the PECVD process we turned our attention to the performance and usability aspects of the Virtual Reactor (Chapters 5 and 6). Here the design considerations were that the simulations should run efficiently both in the *capacity* and in the *capability* mode of the Virtual Reactor. We therefore studied in depth the computational complexity of the PECVD simulations and developed novel parallelization methods to speed up the numerical processes. In this optimization approach we take into account the execution of the Virtual Reactor on tightly coupled (parallel clusters) and loosely coupled (grid-based) computer systems. One of the most challenging problems was porting the parallel modules from homogeneous cluster environments to the heterogeneous resources of the Grid, whilst keeping up the parallel efficiency of the computational components. To solve the load-balancing problem, we developed a theoretical framework and a generic workload balancing technique that takes into account specific parameters of the Grid resources dynamically assigned to a parallel job, as well as the application requirements. We validated the proposed algorithm by applying this technique to the Virtual Reactor parallel solvers running on the Russian-Dutch Grid test-bed. In order to optimize the resource management strategy of mapping the distributed components of the application problem solving environment, we benchmarked the individual components of the Virtual Reactor on a set of diverse Russian-Dutch Grid resources, and extensively studied the behavior of the parallel solvers with various problem types and input data on different resource infrastructures. The results show that the method developed supports dynamic adaptation of the workload over the dynamically changing resources.

Finally, we integrated all the numerical models and computational methods into one Problem Solving Environment. The Virtual Reactor was implemented on the Grid using the Cross-Grid infrastructure and tested against different test-bed configurations. We achieved secure Grid access, resource discovery and registration, Grid data transfer, application initialization, editing physical and chemical properties databases, parameter specification, job submission, distributed simulations and advanced 3D visualization. The foremost conclusion is that the core parallel solver can be efficiently exploited on clusters with high-speed interconnects. The other components of the Virtual Reactor (loosely coupled or fully decoupled) can be distributed across the other Grid resources, thus maximizing the overall

efficiency of the whole application. To increase the efficiency of the solver on heterogeneous resources, the workload balancing techniques developed in the previous chapter was successfully incorporated into the PSE, thus supporting the adaptation of data distribution among the resources according to the network connectivity of the nodes and to the available processing power.

Starting from simplified models, via numerical methods and computer codes, this work has grown into an advanced simulation environment, which has been extensively used in a number of international projects. Recently this work branched into three focused projects aiming at further development of the models, the algorithms and the grid-based environment. Lots of work is planned, and as the history of science shows, solving one problem opens the door to a new one, ever more challenging and exciting..