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Chapter 1. Introduction

1.1. Motivation and scientific challenges

Plasma-Enhanced Chemical Vapor Deposition (PECVD) is nowadays a key sector of the industrial production of silicon-based films, an important material in modern microelectronics, notably transistors, computer chips and solar cells. This industrial sector stimulates research and development of the deposition processes and its physical chemistry. R&D efforts bear on many disciplines: fluid mechanics, chemistry gas-surface interactions to mention but a few. In this context, it must be noted that the engineering and optimization of reactors is much too costly and time-consuming to be left to the sole approach of trial and error, whereby various geometries are tested and then flow rates, temperatures and discharge currents adjusted while growth rates and surface quality are being monitored. Today, advances in numerical simulation offer great perspectives for aiding in the design of new reactors, optimizing the PECVD process and assistance in data reduction and interpretation, etc. The task is not easy, because so many processes need to be accurately taken into account and because expert usage of the most advanced numerical methods is necessary.

Modeling and simulation of the PECVD process is essentially a multidisciplinary endeavor and the state-of-the-art is far from satisfactory. Industry is using codes it has either purchased or developed on its own. Naturally, these codes are proprietary, and they are rarely available to the researchers in universities and research establishments. There also exist commercially-available codes; the latter offer limited flexibility, are not open and are often inefficient. Yet academic research laboratories would greatly benefit from these tools. Indeed, it is precisely in these places that some of the key expertise is found. They have the competence needed to study the complex chemical reactions and to recommend reduced schemes and critical paths, they understand gas-surface mechanisms and can propose and test new precursors. The applied mathematics laboratories are now in a position to cooperate with them fruitfully and to allow them to accomplish great progress, by offering advanced open tools of simulation and parallelization techniques. The work presented in this thesis was launched precisely along this line.

The goal we set out to reach was to develop models and codes for simulation of PECVD technology, to validate them, and to investigate the processes underlying this technology. The models have been validated using data from the literature and from experimental labs partners to the project, most notably Utrecht University, FOM Institute for Plasma Physics and Ioffe Institute of Technical Physics. The codes developed were in turn used to assist the latter in optimizing chamber design and process parameters.

In designing the codes, we followed the modern trend in modeling and simulation technology, departing from rigid simulation codes treating a fixed aspect, towards sophisticated Problem-Solving Environments (PSEs) [1]. These environments are widely

considered to be an essential emerging technology with high impact across all fields of science and engineering. PSEs are especially important to successfully address all kinds of multidisciplinary problems, such as multiphysics multiscale systems, fluid-structure interaction and rapidly developing fields like bio-informatics and other applications where vast amounts of data need to be managed and processed to discover patterns and knowledge contained within them. The research into understanding and improving the complex PECVD processes clearly benefits from such an environment.

The challenge addressed in this thesis is to develop a computationally efficient problem solving environment for PECVD: 'The Virtual Reactor', modeling all the essential multi-physics and multi-chemistry processes.

This work is one of the first attempts to treat 3D flow and 2/3D plasma discharge, thanks to the efficient parallel algorithms and the computational environment taking advantage of Grid computing technologies. This environment has allowed us to solve generic problems posed by modeling complexity and to build a flexible scalable high-performance *Virtual Reactor* for PECVD simulation.

1.2. Background

This subchapter provides a short overview of the PECVD processes, the related modeling and simulation, as well as the simulation environments. More details on the state-of-the-art in these areas can be found in the corresponding chapters.

1.2.1. Modeling and Simulation of PECVD processes

A typical PECVD reactor is a low-pressure chamber of a few liters volume, through which silane (SiH_4), often diluted with molecular hydrogen or argon, is pumped at a low flow rate. A gas mixture enters the reactor at room temperature. In the middle part of the chamber, two parallel electrodes are located (see Fig. 1.1). A substrate for film growth is located at the grounded electrode. To the other electrode, a radio-frequency (RF) oscillating voltage is applied.

A glowing capacitively coupled discharge between the electrodes initiates the ionization and dissociation processes. This leads to the formation of primary silane radicals, which in turn react with each other and with molecules to produce larger radicals. The radicals having free bonds attach to the surface of the substrate, thus composing the actual thin film. To enhance the chemical processes leading to the radicals formation, the substrate is heated to a temperature of around 250 ºC. The products of the chemical reactions that do not deposit are pumped away from the chamber. We should note that together with these products, an expensive silane source gas is also pumped out. One of the goals of the PECVD optimization is increasing the silane consumption ratio.

The quality of the growing films depends, among others, on the percentage of different species contributing to the growth and on the spatial homogeneity of deposition along the substrate. A deeper insight into these aspects of the deposition processes is another goal of the simulation.

A number of intertwined processes occur in a PECVD reactor: the plasma discharge processes (ionization, dissociation, excitation, recombination, attachment, ion

bombardment etc.), convective and diffusive transport, homogeneous (in the bulk) and heterogeneous (on the surfaces) chemical reactions and deposition, heat transfer, etc.

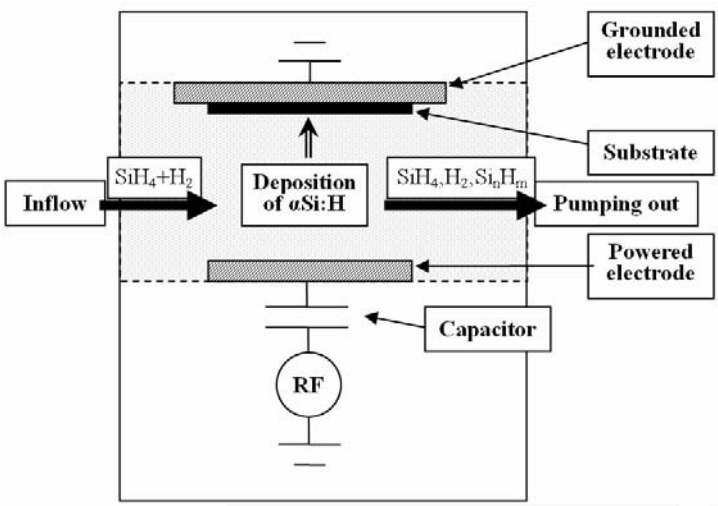

Fig. 1.1. Scheme of a PECVD reactor illustrating the basic principles. The shaded area indicates the discharge zone. In real reactors the geometry is much more complicated. Gases are allowed to flow through the total volume of the chamber

The modeling of these complicated processes can be simplified by noting that we can distinguish the discharge volume, where the plasma processes should be properly simulated, from the whole reactor volume, where only chemical reactions and transport processes should be computed (see Fig. 1.1). The rationale for this simplification stems from the two facts: (1) the energy of the electrons decreases rapidly outside the discharge, thus the high-energy electrons causing dissociation are available only in the discharge volume, and (2) the charged particles are neutralized via ion recombination on a very short distance away from the plasma discharge zone, and therefore can be neglected outside of the discharge volume. Based on these observations, we propose a hierarchical modeling approach with two distinct computational domains where different models and chemical processes shall be considered. Additional details on how this approach works are given in Chapter 2.

To simulate the multidimensional problems, several models have been developed: for 1D, 2D and 3D reactive flow dynamics, and 1D and axisymmetric 2D plasma discharge. Navier-Stokes equations were used to describe the 2D and 3D reactive flow; for the 1D case an original method was developed [2]; for the plasma we used Boltzmann equation together with Poisson equation and particle, momentum, and energy balance equations. For solving the resulting sets of stiff equations, different numerical approaches and algorithms were used.

1.2.2. Computational environment

Traditionally, research codes have been just pieces of computer programs without any user interface, only accessible to their developers, and not to the external user. The only "human" interface was the input and output data files, difficult to compose, understand and interpret. Commercial simulation packages, on the other hand, provide convenient user-friendly interfaces, but do not give enough flexibility in model formulation, choice of equations and numerical methods. One of the steps forward we accomplished was the move from rudimentary programs to easy-to-use research environments.

The importance of fully integrated PECVD simulators (Virtual Reactors) is recognized by various research groups and scientific software companies [3]. The complexity of the simulation necessitates an advanced user-friendly environment to explore the underlying physics and chemistry and associated design characteristics. In order to facilitate efficient data transport, analysis and archiving, as well as computationally efficient parameter-sweeps, we used a Grid-based PSE technology to provide an integrated simulation environment.

Connectivity between distant locations and interoperability between different kinds of systems and resources are some of the most promising characteristics of the Grid. Besides, the computational resources of the Grid provide the required computing power for large-scale simulations and complex visualization and collaborative environments, which are expected to become of major importance to many areas of computational physics.

Within the Virtual Reactor we merged the newly developed distributed interactive simulation and optimization environment [4] with results from the community for scientific computing [5,6] to create an architecture for Grid-enabled PSEs. The PSE considered here is generic in that it can handle High Performance Computing applications (Capability Computing: one parameter setting calculated as fast as possible) as well as High Throughput Computing (Capacity Computing: sweeping various parameter settings) applications.

The middleware we used to build the Virtual Reactor is based on the CrossGrid software system [7] and previous work on integrated environments for computational physics [8]. The CrossGrid pan-European distributed testbed shared resources across sixteen European sites, ranged from relatively small computing facilities in universities, to large computing centers, offering an ideal mixture to test the possibilities of an experimental Grid framework. National research networks and the multi-gigabit pan-European network Geant [9], assured interconnectivity between all sites. Experiments on optimization of load balancing for heterogeneous systems have been conducted on a Russian-Dutch RidGrid testbed.

1.3. Overview of the thesis

The thesis is organized as follows:

Chapter 2 describes the 1D reacting flow and 1D plasma models, discusses the discretization and implementation aspects, and presents the validation of our computational models against experimental data. It also demonstrates simulation results exploring the

influence of PECVD operating conditions on the deposition process and a comparison with analytical results.

Chapter 3 covers the 2D and 3D flow models and implementation, as well as simulation results with the 1D plasma model.

Chapter 4 describes the 2D plasma model and simulation results with the 3D flow.

Chapter 5 introduces the parallel algorithms and load balancing technique for heterogeneous Grid resources.

Chapter 6 details the Grid-based Virtual Reactor problem solving environment.

Chapter 7 brings a summary and conclusions; Chapter 8 gives a summary in Dutch; Chapter 9 offers acknowledgements and Chapter 10 lists the publications by the author.

1.4. References

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