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A virtual reactor for simulation of plasma enhanced chemical vapor deposition

Krzhizhanovskaya, V.V.

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Chapter 4. Modeling and Simulation Part III: 3D Flow and 2/3D Plasma Discharge*

4.1. Introduction

As we concluded in the previous chapter, a 2D or 3D plasma model is essential to capture the spatial inhomogeneity caused by plasma effects. The goal of this Chapter is to combine the 2D plasma model with the 3D flow model introduced in the previous chapter in order to improve the agreement with experiments. The modeling approach for coupling the models stays essentially the same as described in Section 2.1. In the discharge zone, a 2D plasma model is applied and in the entire reactor volume, a 3D reactive flow model is employed (described in Chapter 3).

4.2. 2D Plasma Model

A 2-dimensional (cylindrically symmetric) self-consistent fluid model [3,4] is used for simulation of the RF discharge processes. The continuity equations for electrons, ions and neutrals are solved consistently with the balance equation for the average electron energy and with the Poisson equation for the electric field distribution.

The rates of inelastic electron collisions and the electron transport coefficients are calculated by solving the Boltzmann equation for the electron energy distribution function (EEDF) in the two-term approximation. The EEDF is calculated as a function of the electric field for a given composition of the neutral background density. A look-up table is constructed to obtain the collision rates and electron transport coefficients as functions of the average electron energy, which are used in the fluid model.

While calculating the EEDF, the electric field was assumed to be spatially uniform and stationary. This limitation was compensated in the fluid model by introduction of the spatial and temporal variation of the averaged electron energy.

Further details on this RF discharge model are published in [3,4], including the list of all chemical reactions simulated in the plasma discharge volume (ionization, dissociation, excitation, recombination, attachment).

4.3. Simulation Results

In order to validate the reliability of the model and the usability of the simulation environment we initiated a number of experiments with the ASTER PECVD reactor from the group of Dr. J.K. Rath from Utrecht University [5]. This allowed us to perform detailed studies in a controlled environment. The geometry of the ASTER system is given in Fig.

* Parts of this chapter were published in [1,2]

4.1. It shows the relevant reactor components such as inlet, outlet, electrodes and overall configuration.

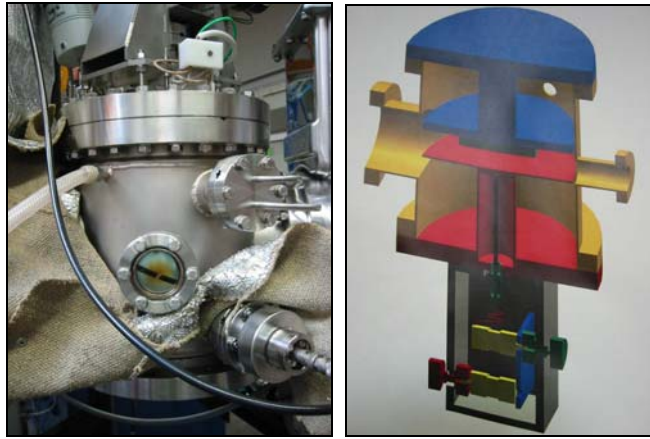


Fig. 4.1. Photo and engineering drawing of the ASTER reactor. The reactor gas chamber has the inner diameter of 200 mm and the height of 280 mm.

We used detailed measurements of the actual geometry of the chamber, substrate and the electrodes as input parameters to our Virtual Reactor. The virtual chamber was constructed from a number of simple blocks, and in each block a regular mesh was generated, as shown in Fig. 4.2.

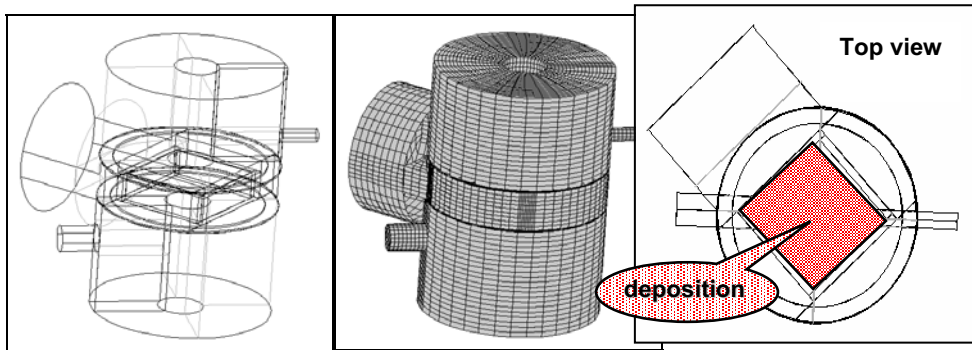


Fig. 4.2. Decomposition of whole computational domain into simple blocks, the generated mesh and the location of the substrate on which the deposition process is taking place.

The initial gas mixture and plasma discharge parameters are chosen corresponding to the real experimental data available [6]. In our comparison the following experimental parameters are used: discharge frequency 50 MHz, applied power 10 W, pressure 0.15 Torr, gas temperature 300 K, substrate temperature 520 K, flow rate 20-60 sccm, inflow mixture composition 50% silane and 50% molecular hydrogen. These conditions were already used in Section 2.7.

Simulation results

We studied in detail the simulation results for the electron distribution as well as the deposition rate on both of the electrodes. In Fig. 4.3 we can clearly see that the area with the maximum electron concentration is located near the edge of the powered (lower) electrode, which corresponds to the edge effects observed in experiments.

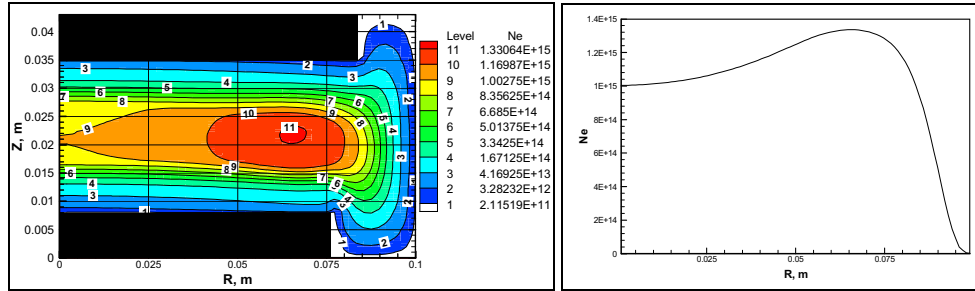


Fig. 4.3. Left: Spatial distribution of the electron concentration. $R=0$ corresponds to the axis of symmetry. N_e is the number of electrons per m^3 . Black plates denote electrodes. Right: electron concentration in the horizontal slice at $Z=0.021$ m (in the middle between the electrodes).

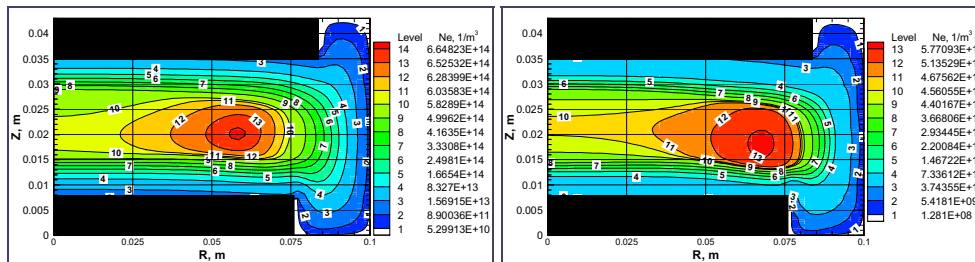


Fig. 4.4. Spatial distribution of electron concentration averaged over RF cycle for different pressures.

We analyzed the spatial distribution of the film thickness. The experimentally observed films have a parabolic variation in thickness, with the minimum in the middle of the substrate, this corresponds to the experimental results (Fig. 4.5).

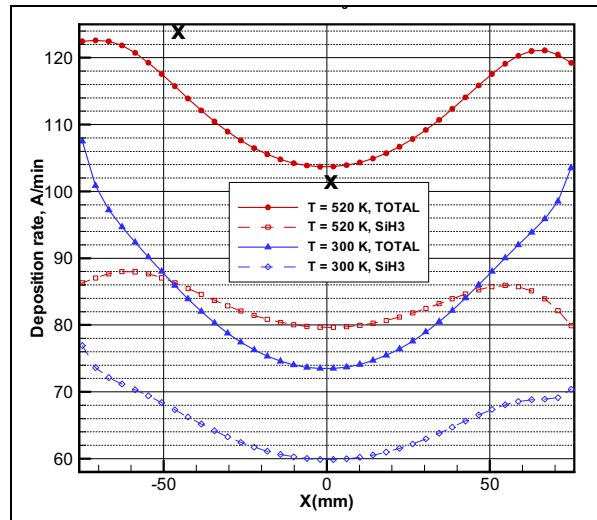


Fig. 4.5. Deposition rate onto the heated (upper) electrode and the 'cold' (lower) electrode. The two experimentally measured values are shown as big crosses 'X'.

4.4. Conclusions

The simulation results are qualitatively in good agreement with respect to the film distribution shape and the observed thickness variation, this variation is more pronounced in the experiment than in the simulation results. 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. We observed a qualitatively good agreement of the simulated results with the experimental data, for instance the correlation of the measured film properties with the simulated ion and radical fluxes towards the substrate [7,8].

These results clearly indicate 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.

We also studied the influence of the reactor configuration and flow rate on the deposition processes with commercial software (CFD-ACE [9]). It was shown that small changes in for instance the inlet and outlet position of the flow significantly affect the uniformity and thickness of the growing film. Detailed studies showed the deposition characteristics are sensitive to the complete experimental parameter space (unpublished results, data not shown).

4.5. References

1. V. V. Krzhizhanovskaya, P.M.A. Slood and Yu. E. Gorbachev. *Grid-based Simulation of Industrial Thin-Film Production*. Simulation: Transactions of the Society for

- Modeling and Simulation International, Special Issue on Applications of Parallel and Distributed Simulation in Industry, January 2005, V. 81, No. 1, pp. 77 - 85
2. V.V. Krzhizhanovskaya, M.A. Zatevakhin, A.A. Ignatiev, Yu.E. Gorbachev, W.J. Goedheer and P.M.A. Sloom. *A 3D Virtual Reactor for Simulation of Silicon-Based Film Production*. Proceedings of the 5th International Bi-Annual Symposium on Computational Technologies for Fluid/Thermal/Structural/Chemical Systems with Industrial Applications, ASME/JSME PVP Conference. San Diego, California USA, July 25-29, 2004. ASME PVP-Vol. 491-2, pp. 59-68, PVP2004-3120. ISBN 0-7918-4686-5
 3. Nienhuis, G.J., Goedheer, W.J., 1999, "Modelling of a large scale reactor for plasma deposition of silicon," *Plasma Sources Sci. Technol.* **8**, pp. 295-298.
 4. Nienhuis, G.J., 1998, *Plasma models for silicon deposition*. PhD Thesis, Utrecht University.
 5. <http://www1.phys.uu.nl/SID/programs/physics%20of%20devices/physdev.html>
 6. Van Sark, W.G.J.H.M., 2001, "Methods of deposition of hydrogenated amorphous silicon for Device applications," in *Handbook of Thin Films Materials*, Vol. 1: Deposition and Processing of Thin Films, Academic Press, San Diego, CA, USA, pp. 1-102.
 7. J.K. Rath, A. Verkerk, M. Brinza, R.E.I. Schropp, W.J. Goedheer, V.V. Krzhizhanovskaya, Y.E. Gorbachev, K.E. Orlov, E.M. Khilkevitch, A.S. Smirnov. Gas phase considerations for the deposition of thin film silicon cells by VHF-PECVD at low substrate temperatures. Accepted at the 33rd IEEE PVSEC.
 8. A. Verkerk, J.K. Rath, M. Brinza, R.E.I. Schropp, W.J. Goedheer, V.V. Krzhizhanovskaya, Y.E. Gorbachev, K.E. Orlov, E.M. Khilkevitch, A.S. Smirnov. Compensation of decreased ion energy by increased hydrogen dilution in plasma deposition of thin film silicon solar cells at low substrate temperatures. Accepted at the Symposium K of the EMRS spring meeting.
 9. <http://www.esi-group.com/products/Fluid-Dynamics/cfd-ace>