# Gas Flow Simulation in a PECVD Reactor

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## 1. Abstract

In this work are presented the gas flow simulation in a home made PECVD-TEOS reactor. We used the FLOTRAN-CFC code of the ANSYS simulator to predict the velocity and temperature curves in the reactor. The results showed high influence of the reactor geometry and the deposition process pressure in the velocity distribution curves.

Key words: PECVD, CFD, gas flow simulation.

## 2. Introduction

The Chemical Vapor Deposition (CVD) process is one of the most important thin film deposition technique used in the integrated circuit technology, because this is a versatile process; allow thickness, structural and composition control, good uniformity and high deposition rate.[1,2,3] The Plasma Enhanced Chemical Vapor Deposition (PECVD) process has the additional advantage that is low deposition temperature (<400°C).[4]

In this work we present the simulation results obtained in a home made cluster tool PECVD system [5,6] aiming at improving the characteristics of the thin film deposition process performed in this reactor.

## 3. Work Presentation

The home made cluster tool system studied in this work was developed to perform doped and undoped silicon oxide deposition. This system has a sample load lock chamber, a PECVD process chamber for undoped and doped silicon oxide deposition; a RTP (Rapid Thermal Processing) process chamber for film annealing and for other rapid thermal processes (Rapid Thermal Oxidation - RTO and Rapid Thermal Nitridation - RTN) under highly controlled conditions, and a central chamber where a robot arm for sample manipulation is located[6].

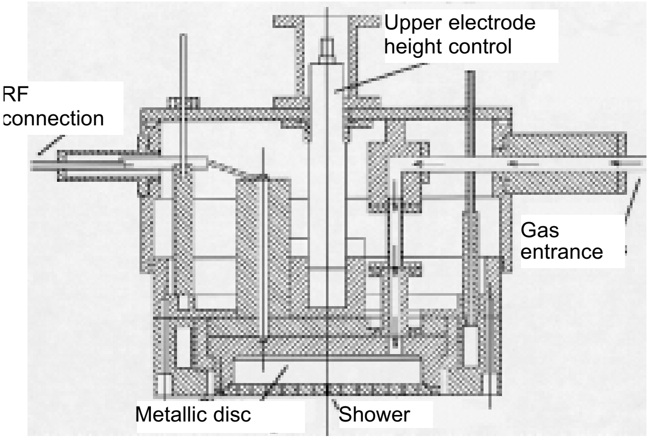


Figure 1: Drawing of the upper electrode showing the gaseous mixture entrance, the metallic disc and the shower position.

The PECVD process chamber has two electrodes. The gas inlet tube that introduces the reagents gases over a first metallic disc. It is used to decrease the gas velocity and to make a gas flux uniformization before the shower. The function of the shower is to obtain uniform gas flow over the substrate. The lower electrode consists in a heated substrate holder. The drawing of the upper electrode in Figure 1 shows the gas mixture entrance the metallic disc and shower position.

It was observed in some deposition conditions, a thickness nonuniformity in the silicon oxide layer, which can be attributed to a gas flow variation inside the reactor. This variation is due to the design of the gas flow system that is not optimized for all deposition conditions. Moreover, the gas flow variation causes a nonuniformity in the gas velocity and gas residence time. The thin silicon oxide films deposited in these conditions present variations in thickness and in the composition.

The focus of this work is to study the behavior of the gas flow through the PECVD reactor in order to optimize the gas flow system. The FLOTRAN-CFD option in the ANSYS simulation program was used to perform the simulations.[7] We simulated the influence of the metallic disc and the shower in the gas velocity distribution, as well as the influence of the process pressure.

For the simulations a two dimensional model of the reactor was drawn. In this model it was considered the gas entrance, the connections to the vacuum pump, the metallic disc and the distribution shower as show in Figure 2. The grid generated in the FLOTRAN-CFD is show in Figure 2 b).

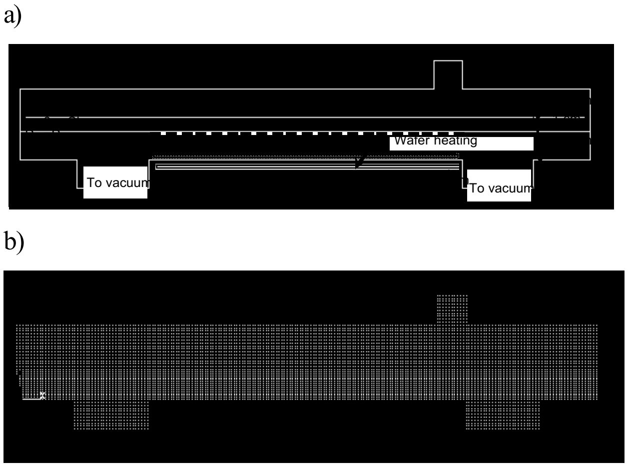


Figure 2: a)2D model of the PECVD reactor showing the degree of freedom used in the simulations, b) computational grid.

The reactor configuration has no axial symmetry, because the gas mixture is introduced laterally in the PECVD chamber (Figure 2). Cartesian coordinates were used.

### 3.1. The Modeling Equations

The analysis of the transport gas flow in a plasma reactor is subjected to the following conditions[8, 9,10]:

1. The mixture of the gas flow is treated as a continuum. Thus, the mean free path of the gas molecules must be shorter than the characteristic reactor dimension which is considered in this case the distance between electrodes.
2. The gases in the plasma reactor are assumed to be ideal, so the ideal gas law can be used.
3. The Reynolds number is small enough to consider the flow laminar.
4. The Mach number is low. Thus, the effects of the pressure variations on the density of the gas mixture can be neglected.
5. The viscous heating of the gas due to the dissipation is neglected since velocity gradients are not large.

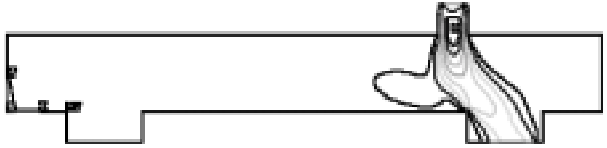
Fluid flow is defined by the laws of conservation of mass, momentum and energy. These laws are expressed in terms of partial differential equations which are discretized using finite elements based techniques[7].

The degrees of freedom applied to the simulated model are the velocity and pressure. The obtained result is VSUM (the vetorial sum of $V_x$ and $V_y$).

## 4. Results And Discussion

### 4.1. Simulation of the Gas Flux in the PECVD Reactor.

a) without distribution plate and gas shower



b) with distribution plate

c) with distribution plate and gas shower

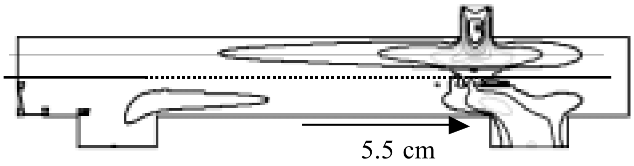


Figure 3: VSUM curves in the PECVD reactor chamber obtained from the simulation with the FLOTRAN-CFD option in the ANSYS simulation program.

In Figure 3, we show the simulation results, as VSUM curves, obtained for the PECVD reactor without the metallic disc and gas shower (a), with the first metallic disc (b) and finally with the metallic disc and gas shower (c). We observe that the first metallic disc modify

The simulated curve of the velocity distribution just over the wafer surface (Figure 4), shows a region where the gas velocity is near zero. This phenomena is due to the change in the gas flux direction caused by the introduction of the first metallic disc associated to the vacuum pump port position. In another words the reactor geometry is the main cause of the near zero velocity region, as show in Figure 5.

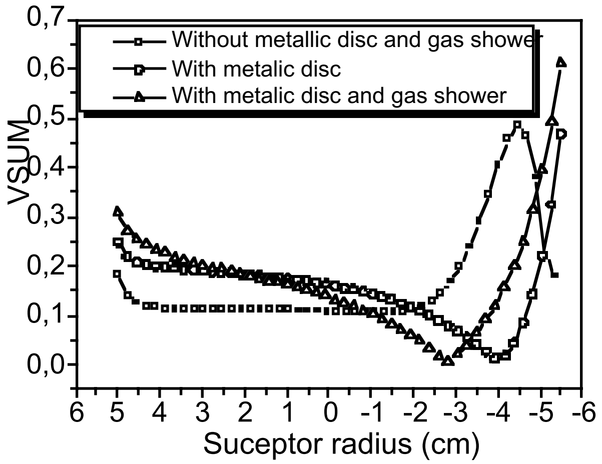


Figure 4: Distribution velocity in the PECVD Reactor chamber.

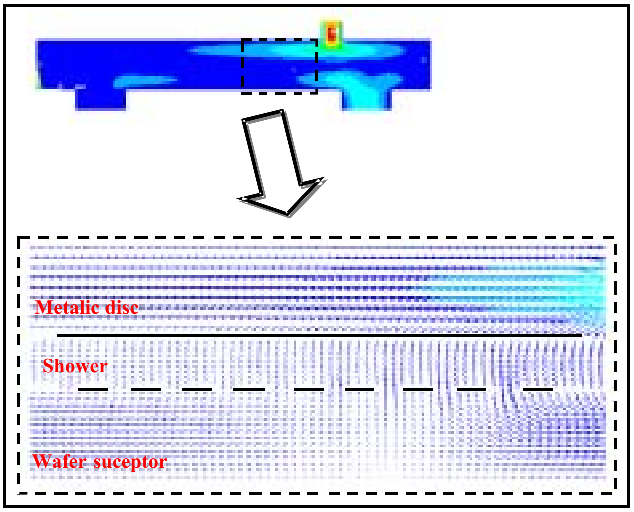


Figure 5: Details of the region where the gas velocity becomes null in the PECVD reactor.

Following these simulations, two different gas flux was analyzed: 155 sccm (which refers to the gaseous mixture: 15 sccm TEOS, 40 sccm $O_2$ and 100 sccm Ar) and 505 sccm (which refers to the gaseous mixture: 5 sccm TEOS and 500 sccm $O_2$). The process pressure, the properties of the gas mixture and velocities used to perform the simulations are listed in the table I.

Table I: Gaseous mixture properties used in the simulation

| P (Torr) | gas flux (sccm) | velocity (cm/s) | ρ (g/cm$^3$) (x10$^{-6}$) | μ (poise) |
|---|---|---|---|---|
| 1 | 155<br>505 | 3.27<br>10.55 | 1.363<br>0.852 | 0.04289<br>0.03581 |

| | | | | |
|---|---|---|---|---|
| 5 | 155<br>505 | 3.27<br>10.55 | 6.84<br>4.273 | 0.04289<br>0.03581 |
| 10 | 155<br>505 | 3.27<br>10.55 | 13.63<br>8.076 | 0.04289<br>0.03581 |

It is observed, in Figure 6, that the simulated velocity (VSUM) is higher when we use a process pressure of 2.5 Torr. We can conclude that in this pressure occurs a change in the diffusion regime inside the chamber.

The simulated velocity distribution curves (Figure 6) do not have a axial symmetry, even using the metallic disc and the shower. We concluded that it is the main reason for the nonuniformity in the silicon oxide deposition process.

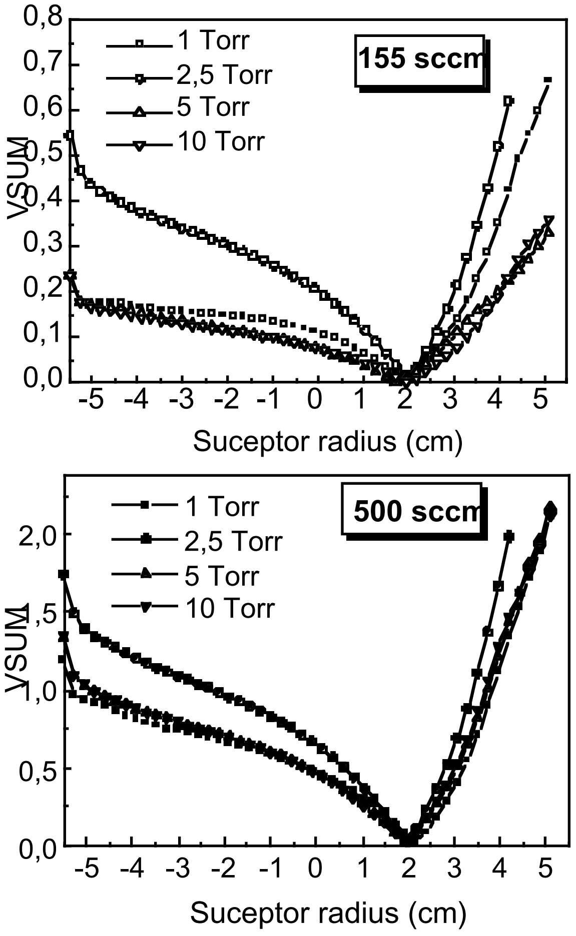


Figure 6**:**Velocity distribution curves (VSUM) selected just over the wafer surface in the reactor for: a) 500 sccm of total gas flux and b) 155 sccm total gas flux.

The gas distribution inside the PECVD reactor was studied. To perform these experiments the reactor was modified changing the external stainless steel walls by a glass cylinder with the same diameter of the original reactor as shown is in Figure 7 a).

A smoke is introduced into the reactor in the same manner as the gas flux during the deposition process. An exhaust device was used to promote the smoke movement inside the reactor. A laser ray was passed through a glass tube that splits the laser ray forming a kind of light plane.

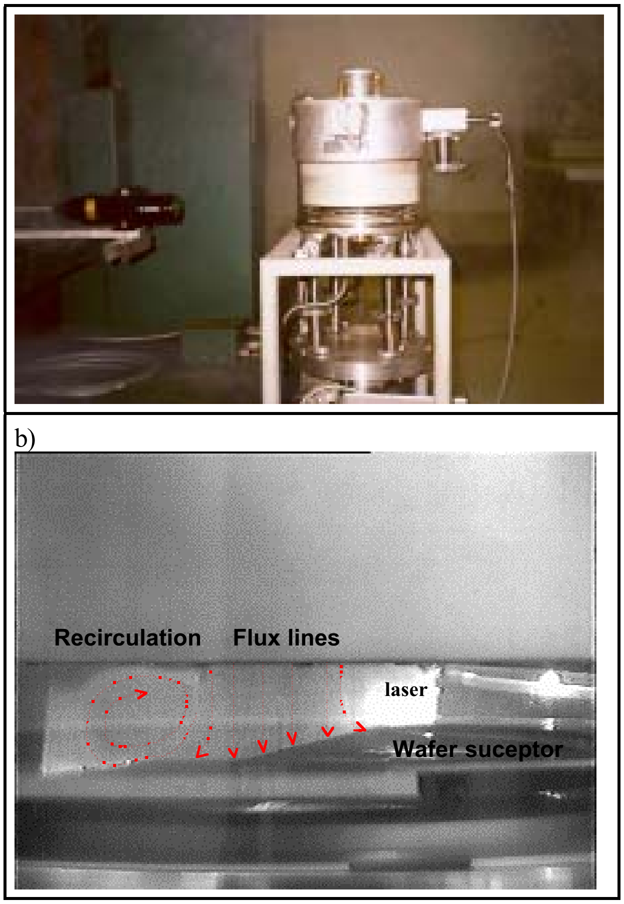


Figure 7: a) The apparatus used to study the gas flux behavior inside the reactor, b) gas flux image.

The incidence of the light plane over the smoke flux reveals the gas flux behavior inside the reactor. The image obtained from this experiment is show in Figure 7 b). It is possible to see that there is recirculation region outside the shower position which agrees well with the simulated VSUM curves showed in Figure 3.

### 4.2. Temperature Influence Simulation

The Figure 8 shows the temperature profiles in the substrate surface. We observed that the temperature profiles have a slight variation over the substrate surface, of around 10 K. Thus, we can conclude that the temperature is uniform over the substrate surface in all process conditions. The nonuniformity is mainly due to gas flux variations.

### 4.3. Distance Between Electrodes Influence Simulation

The influence of the distance between electrodes in the velocity of the gas flow in the PECVD reactor chamber was studied. The gas velocity decreases when increasing the distance between electrodes as observed in the Figure 9 a).

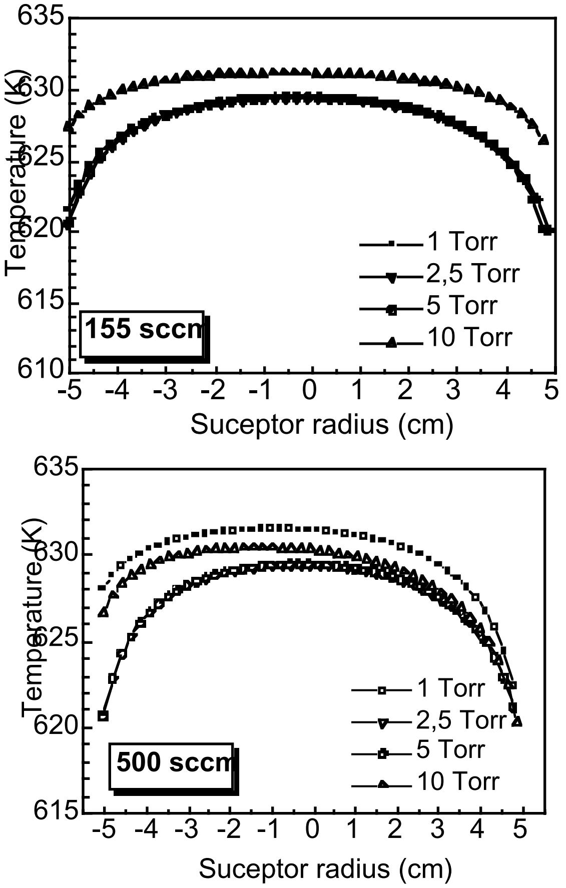


Figure 8:.Temperature Profile

For distances between electrodes larger than 2.0 cm we observe a very low gas velocity distribution. In these conditions we can predict a low quality of the deposited layer, because the residence time increases, which promotes the vapor phase reaction during the deposition process as well as the film deposition on the reactor walls. The distance between electrodes has almost no influence in the temperature profiles as we can observe in Figure 9 b).

## 5. Conclusions

We concluded that there is an influence of the reactor geometry in the gas flow. We also showed that the temperature distribution in the region near the wafer does not depend on pressure and velocity, but depends only on the gas characteristics.

Modifying the gas flow entrance we change the gas velocity profile and the velocity distribution becomes independent of the process pressure. However, in our simulations it was not possible to avoid the zero velocity regions. More studies concerning this are necessary.

The reactor geometry has a great influence in the gas flow behavior. The gas mixture temperature distribution in the region near the wafer depends only of the gases characteristics.

The simulations results of a new geometry of the PECVD chamber showed that it is necessary to modify the chamber in order to improve the uniformity of the deposited thin film.

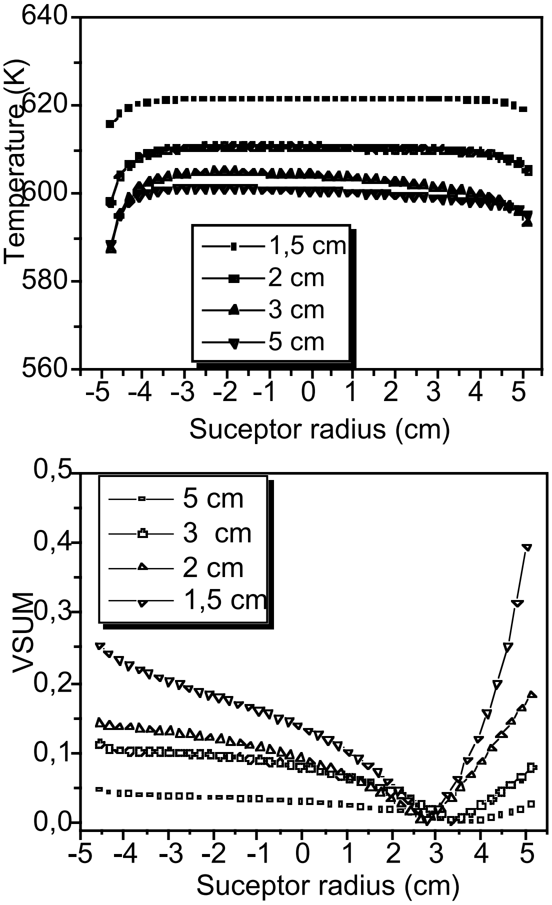


Figure 9: a) Velocity Profile, b) Temperature Profile.

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