LRP 642/99 July 1999

# A gas flow uniformity study in large-area showerhead reactors for RF plasma deposition

L. Sansonnens, A.A. Howling, Ch. Hollenstein

ISSN 0458-5895

# A gas flow uniformity study in large-area showerhead reactors for RF plasma deposition

L Sansonnens †, A A Howling and Ch Hollenstein

Centre de Recherches en Physique des Plasmas, Ecole Polytechnique Fédérale de Lausanne, PPH – Ecublens, CH-1015 Lausanne, Switzerland

**Abstract.**

A simple one-dimensional model for plasma deposition in a rectangular showerhead reactor with single side pumping has been developed in order to explain the mechanisms which yield uniform deposition using this gas flow configuration. Although the flow velocity increases linearly with distance towards the pumping side, the solution of the transport equations for the neutral species shows that their number densities are constant throughout the reactor. Consequently, the plasma and surface deposition reactions are independent of position in any arbitrarily-large area showerhead reactor.

PACS numbers: 52.75.Rx, 81.15.Gh, 52.80.Pi

Short title: Gas flow uniformity in large-area reactors

July 30, 1999

† Present address: CSIRO Telecommunications and Industrial Physics, PO Box 218, Lindfield, NSW 2070, Australia. E-mail address: Laurent.Sansonnens@epfl.ch

## 1. Introduction

Plasma assisted deposition or etching of thin solid films such as amorphous silicon or silicon oxide has widespread applications, especially in the field of photovoltaic solar cells and thin film transistors for flat screen production. Industrial applications require high deposition rates over large areas (35 cm $\times$ 45 cm or more for flat screen applications) with a layer thickness uniformity to better than $\pm$ 5% for flat screens and about $\pm$ 10% for solar cells.

The radio-frequency parallel-plate plasma reactor is the most commonly used configuration in industry for large area applications. In the design of a reactor, special care must be taken in order to obtain the required film thickness homogeneity. Some considerations include the configuration of the RF electrode connections [1], powder contamination [2], and electrode topology [3]. This paper is concerned with the gas flow distribution in the reactor, which is another key parameter that will affect the deposition uniformity. Essentially two types of gas flow arrangement have been studied and are currently used in industry: In one case, the gas flow enters the reactor through one side and is pumped through the opposite side [4, 5, 6] and in the other case, the gas flow is uniformly distributed in the reactor by a showerhead electrode, and is still pumped through one side of the reactor [6, 7, 8]. In this paper, the first configuration will be referred to as the longitudinal flow reactor, and the second configuration as the showerhead reactor.

Dollet *et al* [4] and Park *et al* [5] have shown that uniform deposition rate and film composition are difficult to achieve in the longitudinal flow reactor configuration. The reason is that the working gas is more and more depleted in the direction of the gas flow and therefore, the composition of the gas depends on the position in the reactor. This non-uniformity of the gas composition induces inhomogeneities in the deposition rate and in the film composition. They have shown that the uniformity can be improved by on-off power modulation [5, 9]. But in this case, the time on and the time off will depend on the other operation parameters such as the pressure, input gas flow or power dissipated in the plasma, and on the reactor dimensions. Any change in one of these parameters will then require the adjustment of the other parameters in order to preserve the uniformity. Therefore, this method is not really well adapted for the upscaling of the reactor or for a wide domain of operation.

Calculations performed by Caquineau and Despax [6] have shown that the uniformity can be greatly improved by using the showerhead reactor geometry. The models used for these calculations solve the transport equations for the neutral species in two-dimensional geometry and include the complex chemistry that occurs in the plasma. Due to its complexity, this model does not clearly show what are the mechanisms which make the deposition rate uniform in the showerhead reactor. On one hand, it might

seem obvious that if the gas is uniformly distributed in the plasma, the uniformity of the deposition rate will be improved. But on the other hand, the fact that the gas is distributed over the whole electrode area implies that the gas flow is higher near the pumping side than on the opposite side of the reactor. The residence time of the gas in the reactor therefore depends on position and it is not intuitively clear why the deposition is more uniform with a showerhead.

In this paper, we present a simplified analysis of the deposition mechanism in a rectangular showerhead reactor. The model is based on a one-dimensional approximation for the transport of the neutral species in the reactor and it is purposely limited to the minimum number of chemical reactions necessary to describe Plasma Enhanced Chemical Vapor Deposition (PECVD), although the treatment remains valid if more reaction steps are included. The aim of this model is not to replace a full two-dimensional calculation involving the complex plasma chemistry that occurs in a real case, but to show clearly what is the reason that makes the deposition rate uniform in the showerhead geometry.

## 2. Model

Figure 1 shows a schematic of the system studied. The plasma reactor consists of two rectangular electrodes separated by an electrode gap $L_z$ which is small compared to the electrode lateral dimensions $L_x$ and $L_y$, with $L_x$ the length of the reactor in the direction of the flow towards the pump, and $L_y$ the width of the reactor. The working gas is introduced through a uniform showerhead located in the top electrode and is pumped on one side of the reactor through a grid which is used to confine the plasma. On the other three sides of the reactor, the gas and the plasma are confined by walls. This reactor corresponds, for example, to the reactor described in [1] for amorphous silicon deposition. In this specific case, the electrode gap $L_z$ is 2.5 cm and the electrode dimensions are 57 cm long ($L_x$) by 47 cm wide ($L_y$). The pressure range is typically from 0.2 to 1 mbar and the total input gas flow is between 50 to 500 sccm. The input gas can be pure silane or silane diluted in an inert gas or hydrogen.

The focus of this paper is to show the uniformity of the deposition rate in a showerhead reactor type and not to give a detailed model of deposition for a specific case. Therefore, the deposition process is represented by the two following simple reactions, which are the minimum necessary to describe a general PECVD process with no loss of generality:

$$\text{plasma dissociation} : AB_2 + e \xrightarrow{k_d} AB + B + e \tag{1}$$

$$\text{surface reactions} : AB + surface \xrightarrow{k_s} A_s + B \tag{2}$$

The precursor molecules $AB_2$ are partially dissociated in the plasma by electron-impact (reaction (1), with rate constant $k_d$) to produce reactive radicals $AB$ and $B$. The radicals are transported in the reactor by diffusion and convection and can react with the surfaces to produce a solid film ($A_s$, where the subscript $s$ refers to a solid product) and volatile product ($B$) (reaction (2)). The deposition reaction is a surface reaction, but the reaction rate constant $k_s$ is expressed as a homogeneous volume reaction rate [10]. $k_s$ then includes the effect of the diffusion of the radicals towards the surfaces, and the surface-to-volume ratio.

In order to further simplify the analysis, the following assumptions are also introduced and discussed below:

1. The continuum approximation is valid.

2. The species concentration is independent of height $z$ between the two electrodes and the flow velocity profile is flat and directed in the pumping direction (one-dimensional approximation).

3. The system is isobaric and isothermal.

4. The electron density and energy are spatially uniform and the reaction rate with the surface is uniform.

5. The system operates in a steady-state mode.

The first assumption means that the pressure is high enough for the particle mean free path to be much smaller than the smallest reactor dimension and, therefore, that the fluid equations are valid for describing the particle transport.

The second assumption is, in fact, in contradiction with the principle of the showerhead geometry, since the gas enters the reactor through the top electrode and is pumped through one side of the reactor; this would clearly give a two-dimensional fluid flow. Nevertheless, for a reactor with a large aspect ratio (ie small electrode gap and long electrodes), the velocity of the flow in the pumping direction, after a short distance from the back wall, is larger than the vertical velocity and therefore we can, to a first approximation, neglect the vertical flow velocity. In the real situation, the flow in the direction of the pumping is also not flat but has a parabolic velocity profile and the density profile between the electrodes for the different species is not completely flat. The fact that the working gas is introduced through the top electrode and the fact that the radicals deposit on the surfaces can introduce an interelectrode density gradient. Nevertheless, the interelectrode gradient density and the effect of the parabolic velocity profile will remain small when the vertical Peclet number $P_e$, defined by $P_e = vL_z/D_i$ (where $v$ is the flow velocity and $D_i$ the diffusivity of the species $i$), is much less than 1. This is generally the case for a small electrode gap and relatively high diffusion rate and therefore the one-dimensional model can be used as a first approximation to the real situation.

The third assumption implies a negligible pressure drop along the reactor and a

thermal conductivity high enough to maintain a uniform temperature. For viscous flow, the pressure variation along a rectangular shower type reactor with pumping through one side is given by the expression:

$$\frac{\Delta P}{P} = \frac{6\eta V_0 L_x^2}{L_z^3 P} = \frac{6\eta L_x}{L_y} \frac{Q}{L_z^3 P^2} \tag{3}$$

where $P$ is the pressure inside the reactor, $\eta$ is the gas viscosity, $V_0$ is the downward gas velocity at the showerhead and is related to the total flowrate $Q$ by $Q = V_0 P L_x L_y$. For silane at 200°C, $\eta = 1.2\,10^{-5}$ kgm$^{-1}$s$^{-1}$ and for the geometry described above, a pressure variation $\Delta P/P$ of 2 % is obtained for a total flowrate of 500 sccm at 0.2 mbar. This pressure variation will be smaller for lower flowrates and/or higher pressures. The pressure drop due to the flow velocity,

$$\frac{\Delta P}{P} = \frac{3\rho V_0^2 L_x^2}{L_z^2 P} = \frac{3\rho}{L_y^2 L_z^2} \frac{Q^2}{P^3} \tag{4}$$

using Bernoulli's principle ($\rho$ is the gas density), is one order of magnitude smaller and can be neglected in comparison with the effect of viscosity.

The fourth assumption means that the reaction rates are uniform along the reactor. In reality, the electron density and energy have strong interelectrode gradients which introduce non-uniform interelectrode reaction rates, but for a small interelectrode gap and rapid diffusion, the Damkohler number $D_a$ defined by $D_a = k_d n_e L_z^2 / D_i$ will remain small and therefore the reaction rate can be averaged across the interelectrode space in order to obtain a one-dimensional model.

The last assumption implies that the system can be described with time-independent equations. In the case of rf excitation, only the electrons are sufficiently mobile to follow the rf electric field variation and therefore the time-independent model can be applied for the heavy particle transport. In this case, the reaction rate $k_d$, depending on the electrons, must be averaged over one rf cycle.

Using the above assumptions, the conservation equations for the different neutral species become:

$$\frac{d}{dx}(n_{AB_2} v(x)) = D_{AB_2} \frac{d^2 n_{AB_2}}{dx^2} + \phi - k_d n_e n_{AB_2} \tag{5}$$

$$\frac{d}{dx}(n_{AB} v(x)) = D_{AB} \frac{d^2 n_{AB}}{dx^2} + k_d n_e n_{AB_2} - k_s n_{AB} \tag{6}$$

$$\frac{d}{dx}(n_B v(x)) = D_B \frac{d^2 n_B}{dx^2} + k_d n_e n_{AB_2} + k_s n_{AB} \tag{7}$$

where $n_i$ ($i = AB_2, AB$ or $B$) and $D_i$ are respectively the density and the diffusivity of species $i$. In equation (5), $\phi$ represents the source term of the working gas. In the one

dimensional approximation, this term is a constant volume source term and is given by the ratio of the total flux through the showerhead divided by the volume of the plasma reactor. $v(x)$ is the fluid velocity averaged over the electrode gap.

As the system is assumed isobaric and isothermal, the total density $n_t$ is constant across all the reactor:

$$n_t = n_{AB_2} + n_{AB} + n_B = const. \tag{8}$$

## 3. Solution and discussion

Equations (5) to (8) are a system of four independent differential equations with four unknowns ($n_{AB_2}$, $n_{AB}$, $n_B$ and $v$). Therefore, for an appropriate set of boundary conditions, this system will have a unique solution.

If the deposition on the vertical walls of the reactor is neglected, the boundary conditions for the densities are:

$$\frac{dn_i}{dx} = 0 \quad \text{at} \quad x = 0 \quad \text{and} \quad x = L_x \tag{9}$$

and the boundary condition for the velocity is:

$$v = 0 \quad \text{at} \quad x = 0. \tag{10}$$

With this set of boundary conditions, it is easily verified that the solution of the differential equation system is given by:

$$v(x) = a\,x \quad \text{and} \quad n_i = constant \quad \forall i \tag{11}$$

where $a$ is a constant. The density of each species is constant over the whole reactor, there are no density gradients and so the diffusion terms in equations (5) to (7) are zero. Since the deposition rate is proportional to $k_s n_{AB}$, and $n_{AB}$ is constant along the reactor, the solution of the one-dimensional model shows that the showerhead geometry, combined with pumping along one side, gives a uniform deposition rate. As mentioned in the introduction, this uniformity is not self evident because, on a molecular level, the residence time of the working gas is not the same over all the reactor volume. To understand the uniformity of this showerhead and single-side pumping configuration, we must consider the collective or fluid behavior of the flow of molecules: The net volumetric flux of species $i$ leaving an elemental volume, thickness $dx$, at position $x$ is $n_i dv/dx$. Using equation (11), it follows that the net loss rate of each molecular species due to the flow is therefore constant in all the reactor. The term $a = dv/dx$ can be seen as an effective inverse residence time for the fluid, and the term $n_i dv/dx$ is the effective pumping loss rate of the molecule of type $i$ in the showerhead geometry. For each species, this loss is balanced by the constant source rates of the working gas, $\phi$, and the plasma dissociation products. This can be seen from the conservation equations

(5) to (7) which, on substitution of equation (11), are all independent of $x$. The fact that all of these terms are constant along the reactor is the key factor that makes the deposition rate uniform in the showerhead geometry. For the case of longitudinal flow, where $\phi = 0$ in equation (5), the working gas density $n_{AB_2}$ necessarily decreases along $x$, with the consequence that density gradients are introduced into the solution for all the gas species, resulting in a non-uniform deposition rate.

The chemical model used in this paper contains only three kinds of neutral particles and two reactions to describe a deposition process; this is not sufficient to represent the details of the complex chemistry which occurs in a real case. However, the solution obtained for this simple model remains valid for more complicated models with more species and more reactions, provided that all the reaction rates remain constant along the reactor. The same model can also be applied to describe the uniformity of plasma etching in the showerhead geometry. The plasma and surface reactions, summarised in equations (1) and (2), are therefore independent of position in any arbitrarily-large showerhead reactor with single side pumping, which justifies the use of particularly simple zero-dimensional models, as in reference [11].

The uniformity of the showerhead configuration has been explained starting from the basis of a one-dimensional model which necessitated assumptions which will not always be valid for a real case. A more complete two-dimensional model has been developed by Caquineau *et al* [6]. The results of their calculations show that the showerhead geometry improves the uniformity of the deposition in comparison with the longitudinal flow geometry, but their calculations also show that some inhomogeneities still exist in the showerhead configuration. The major cause of these inhomogeneities is due to the fact that the deposition occurs also on the lateral walls of the reactor. This lateral deposition, which has been neglected in the present one-dimensional model, decreases the radical density in the vicinity of the walls and results in a non-uniform radical density distribution and deposition rate. Nevertheless, the calculations also show that these non-uniformities remain confined close to the wall for large area reactors with small electrode gap, and therefore the results of the one-dimensional model in this paper remain valid for describing the effect of the showerhead gas distribution in the central part of the reactor, away from the walls.

As mentioned in section 2, the uniformity of a rectangular showerhead reactor has been demonstrated assuming a negligible pressure drop across the reactor. According to (3), the pressure variation due to the viscous flow between the electrodes increases with the total flowrate and decreases with the pressure and electrode gap. Since the flowrate is in general proportional to the area of the reactor, we can distinguish two classes of reactor: 1) Small reactors (smaller than 0.5 $m^2$): Unless operated at low pressure and high flowrate, the variation of the pressure remains small and the uniformity of the deposition is affected principally by the deposition on the lateral walls. 2) Large

reactors: In this case, the pressure variation across the reactor can become large and cause non-uniform deposition. Therefore, in the design of a large reactor, special care must be taken to minimise the pressure drop across the reactor. Since $\Delta P/P$ is inversely proportional to the cube of the electrode gap, one possibility to decrease $\Delta P/P$ is to increase the electrode gap. Another possibility is to pump through two opposite sides (not adjacent sides) of the reactor. In that case, $\Delta P/P$ is reduced by a factor 4 in comparison with a reactor with pumping along a single side; the principle of uniformity of the showerhead is not altered since by symmetry the gas flowrate is zero at the midplane and, therefore, this configuration is equivalent to two reactors with pumping along one side placed back-to-back.

By using cylindrical co-ordinates for equations (5) to (7), the gas distribution appropriate for uniform deposition (or etching) in a circular electrode parallel-plate reactor is also shown to be a uniform showerhead, with pumping over the whole circumference.

## 4. Conclusion

A one-dimensional model for plasma deposition in a showerhead reactor with single-side pumping has been developed in order to explain the mechanisms which yield uniform deposition using this gas flow configuration. The solution of the transport equations shows that in the one-dimensional approximation, the density of each neutral species is constant along the reactor and the flow velocity increases linearly with distance towards the pumping side. The plasma and surface reactions are then seen to be independent of position in any arbitrarily-large showerhead reactor with single-side pumping, which justifies the use of simple zero-dimensional models to describe the plasma chemistry in these reactors.

The present model is only a simplification of a real deposition system and more complicated two- or three-dimensional models are necessary to show, for example, the effect of deposition on the lateral walls on the deposition uniformity. However, the essential features of the showerhead plasma reactor operation are explained by the one-dimensional model.

## Acknowledgments

We thank Dr. J. P. M. Schmitt for his advice and suggestions. This work was funded by Swiss Federal Research Grant BEW 9400051 and partly supported by the Swiss National Foundation.

## References


[1] Sansonnens L, Pletzer A, Magni D, Howling A A, Hollenstein Ch and Schmitt J P M 1997 *Plasma Sources Sci. Technol.*, **6** 170

[2] Hollenstein Ch, Howling A A, Courteille C, Dorier J-L, Sansonnens L, Magni D and Muller H 1998 *Mater. Res. Soc. Symp. Proc.* Vol 507 (Pittsburgh, PA: Materials Research Society) p 547

[3] Meiling H, Van Sark W G J H M, Bezemer J and Van der Weg W F 1996 *J. Appl. Phys.*, **80** 3546

[4] Dollet A, Couderc J P and Despax B 1995 *Plasma Sources Sci. Technol.*, **4** 94

[5] Park S-K and Economou D J 1991 *J. Electrochem. Soc.*, **138** 1499

[6] Caquineau H and Despax B 1997 *Chemical Engineering Science*, **52** 2901

[7] Economou D J, Park S-K and Wiliams G D 1989 *J. Electrochem. Soc.*, **136** 188

[8] Park S-K and Economou D J 1990 *J. Electrochem. Soc.*, **137** 2624

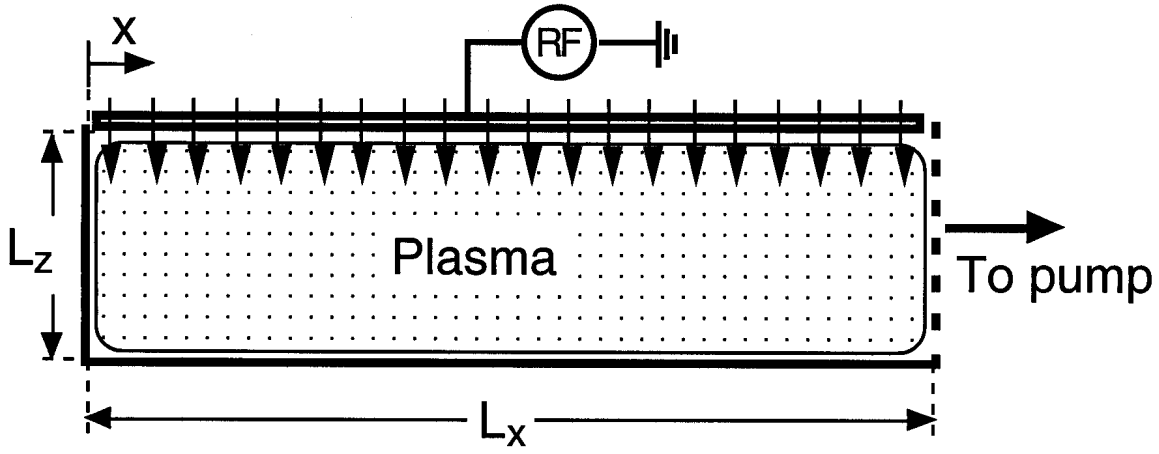
[9] Dollet A, Layeillon L, Couderc J P and Despax B 1995 *Plasma Sources Sci. Technol.*, **4** 459

[10] Park S-K and Economou D J 1990 *J. Electrochem. Soc.*, **137** 2103

[11] Sansonnens L, Howling A A and Hollenstein Ch 1998 *Plasma Sources Sci. Technol.*, **7** 114

## Figure captions

**Figure 1.** Schematic cross-sectional side view of a showerhead type reactor. The working gas is introduced through the top electrode and the residual gas is pumped through one side of the reactor. In this example, the showerhead is the RF electrode, and the bottom electrode, the three vertical walls and the pumping grid are all grounded.


x
RF
Plasma
To pump
$L_z$
$L_x$