

DESIGN, SIMULATION, AND EXPERIMENTAL TESTING OF A SPATIALLY CONTROLLABLE CVD REACTOR

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Abstract: Most conventional chemical vapor deposition systems do not have the spatial actuation and sensing capabilities necessary to control deposition uniformity, or to intentionally induce nonuniform deposition patterns for single-wafer combinatorial CVD experiments. In an effort to address this limitation, a research program is underway focusing on developing a novel CVD reactor system that can explicitly control the spatial profile of gas-phase chemical composition across the wafer surface. This paper discusses the development of a simulator for the three-segment prototype that has recently been constructed and the results of preliminary experiments performed to evaluate the performance of the prototype in depositing tungsten films. *Copyright © 2003 IFAC*

Keywords: Semiconductor processing; Chemical vapor deposition; Distributed parameter systems; Simulation.

1. INTRODUCTION

Chemical Vapor Deposition (CVD) is one of the essential processes in semiconductor manufacturing because of its ability to deposit thin smooth films conformally onto submicron-scale features. CVD processes have evolved together with the semiconductor industry, from early bell-jar CVD reactors to the current cold-wall single-wafer reactor (Xia *et al.*, 2000). Although current conventional CVD reactors produce thin smooth films successfully, their configurations lack the 2-dimensional spatial controllability necessary to counteract non-uniformity generators such as reactant depletion.

Significant research effort has been put into improving uniformity of deposited thin films (Wang *et al.*, 1986; Moffat and Jensen 1988; Kleijn *et al.*, 1989; Moslehi *et al.*, 1995; van der Stricht *et al.*, 1997; Yang *et al.*, 1999; Theodoropoulos *et al.*, 2000). Most of these studies have focused on optimizing the process operating parameters (gas

input rate, wafer temperature, and reactor pressure) and apply to reactor configurations that do not allow any adjustments to their overall geometry (Wang *et al.*, 1986; Moffat and Jensen 1988; Kleijn *et al.*, 1989; Moslehi *et al.*, 1995; van der Stricht *et al.*, 1997). Because current configurations of CVD reactors mostly lack precise control actuators for gas delivery to the wafer surface, the spatial control of film characteristics becomes limited by inflexible CVD reactor configurations. While some research has focused on distributing precursor gases across the wafer surface with pre-specified spatial variation (Yang *et al.*, 1999; Theodoropoulos *et al.*, 2000), the reactor designs were mainly motivated by the goal of decreasing gas phase reactions in MOCVD processes using designs that separate precursors to improve film uniformity.

As a response to these perceived CVD reactor design shortcomings, we have developed a novel CVD reactor intended to improve across-wafer 2-dimensional controllability. This new CVD reactor introduces a segmented showerhead design featuring

individually controllable gas distribution actuators, a design that reverses the residual gas flow by directing it up through the showerhead (henceforth referred to as the reverse-flow design), and sampling ports for in-situ gas sampling.

In this paper, we describe the proof of this novel design concept by simulation and a sequence of experiments performed using a prototype reactor. We refer to this design as the Programmable CVD Reactor Concept because of the potential of real-time control of gas phase composition across the wafer surface. An illustration of the three-zone prototype Programmable CVD reactor is shown in Fig. 1.

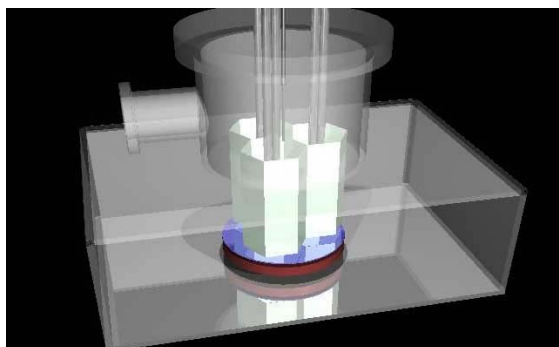


Fig. 1. The Programmable CVD reactor illustrating the segmented showerhead structure.

2. CVD REACTOR PROTOTYPE DESIGN

The major design feature of the Programmable CVD reactor is its segmented showerhead. A schematic diagram of the reactor is shown in Fig. 2.

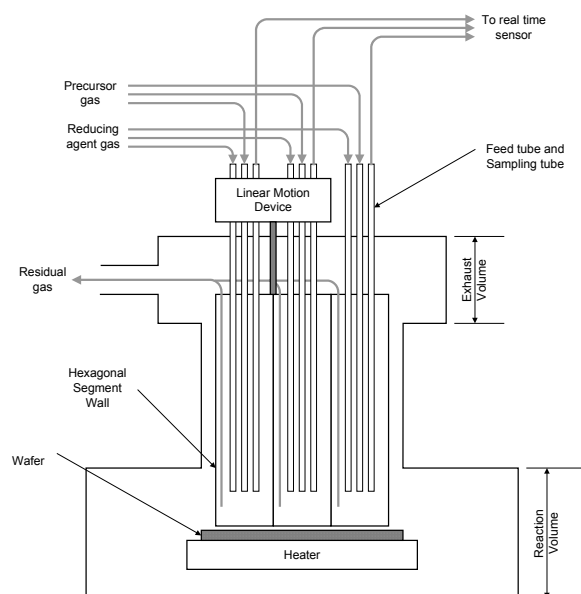


Fig. 2. Schematic diagram showing a vertical cross-section of the Programmable CVD reactor and its feed gas delivery system.

The effect of the segmented showerhead design is to discretize the region above the wafer surface into individually controllable regions. Because each segment is fitted with separate feed gas lines, the precursor gas composition in the area of wafer

surface corresponding to each segment can be individually adjusted.

To enhance film uniformity in the wafer area corresponding to each segment and to reduce interaction between segments, residual gas is recirculated up through each segment of the showerhead and mixed in a common exhaust volume above the showerhead honeycomb structure (Fig. 3). The reverse-flow of exhaust gas means diffusional transport dominants in the region above the wafer and below the bottom of the showerhead segments. This design feature increases the controllability of across wafer gas composition relative to conventional CVD reactors, which normally draw residual gas across the wafer surface (e.g., Moslehi *et al.*, 1995).

Showerhead/wafer spacing is controlled with the linear motion device shown in Figure 2. The sampling tube of each segment can be used to transport a small amount of gas to a real time in-situ sensor, such as a mass spectrometer. From the residual gas analysis of each segment, approximate film thickness and the composition of film deposited on each area corresponding to each segment can be determined. Also, this sampling tube and sensor can be used to diagnose process operation during a deposition run.

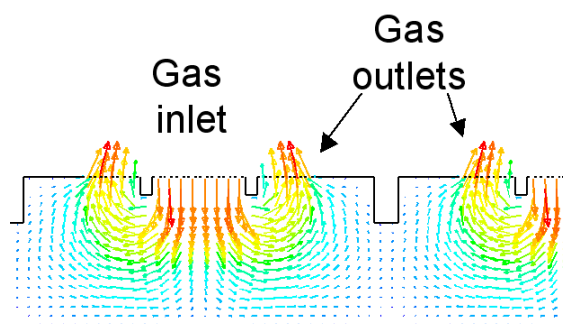


Fig. 3. Periodic gas flowfields generated by the recirculating showerhead design.

To test the feasibility of the Programmable CVD concept, we have constructed a prototype reactor by modifying one reaction chamber of an Ulvac-ERA1000 CVD cluster tool. The Ulvac-ERA1000 CVD cluster tool located on the University of Maryland's campus is a commercial CVD tool used for selective tungsten deposition. In its original configuration, the hydrogen reducing gas entered through a quartz showerhead above the wafer; wafer heating was provided by a ring of heating lamps above the showerhead. As part of the programmable reactor modification, substrate heating was used in place of lamp heating, and the quartz showerhead was replaced by a new assembly consisting of a three-segment honeycomb structure equipped with two feed tubes and one sampling tube per each segment. (Fig. 4.)

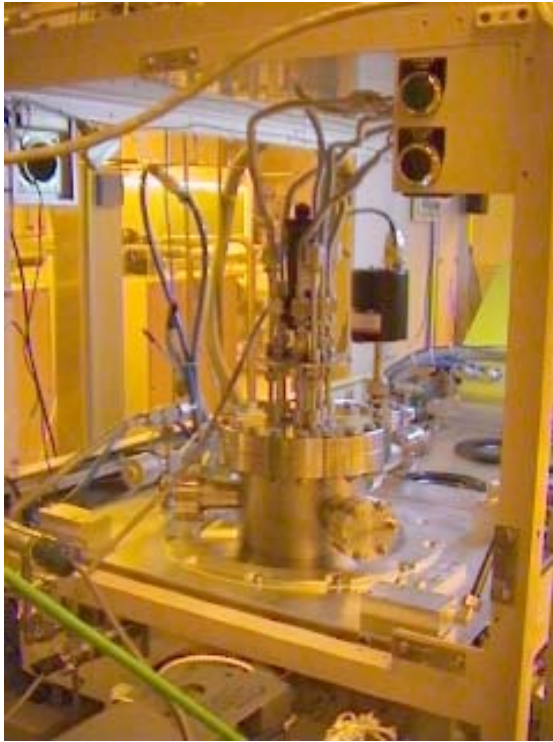


Fig. 4. A photograph of the three-zone prototype showerhead mounted on the Ulvac reactor chamber.

The prototype system is designed to deposit tungsten films using the hydrogen reduction process; this deposition process was chosen to test the prototype reactor because the Ulvac reactor originally was designed for tungsten deposition, and the reactions for tungsten deposition by hydrogen reduction have well known mechanisms and rate expressions (Arora and Pollard, 1991; Kleijn 2000; Kleijn *et al.*, 1991; Kleijn and Werner, 1993). Additionally tungsten deposition remains a commercially important manufacturing process (Ireland, 1997).

2. PROTOTYPE EXPERIMENTAL TESTS

A number of initial experiments were performed using the three zone prototype to validate the design assumptions and collect data for developing a detailed process simulator. Typical operating conditions for the first experiments consisted of a 0.5 torr chamber pressure, a wafer temperature of 350°C, and 20 minute deposition times. In all cases where the showerhead/wafer spacing was small (e.g., 1mm), distinct hexagonal film patterns were produced (Fig. 5), and as anticipated, the pattern became more diffuse as the showerhead/wafer increased.

In one particular set of experiments, pure Ar was fed to Segment 1 at a flowrate of 50sccm; 50sccm of WF_6 was fed to segment 2, and 50sccm of H_2 was fed to segment 3. The film thickness in the region below each segment was determined by sheet resistance measurements using a four-point probe; the interpolated results are shown in Fig. 6. While some W deposition should take place directly under Segment 2 (where pure WF_6 is fed) due to the Si reduction mechanism, it is interesting to note that

some W deposition takes place under the remaining two segments. An explanation for this phenomenon is presented in the following sections on segment simulator development.

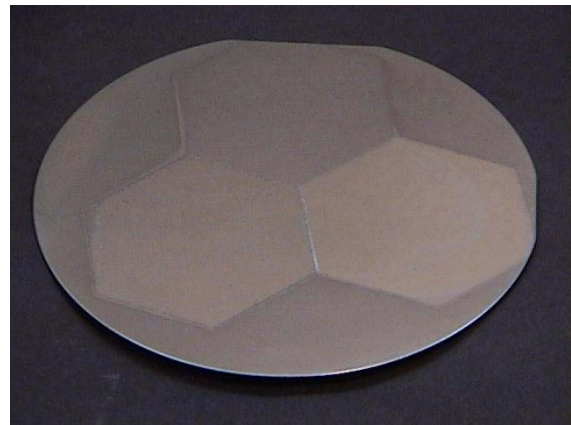


Fig. 5. Typical tungsten deposition pattern produced by the prototype Programmable CVD reactor.

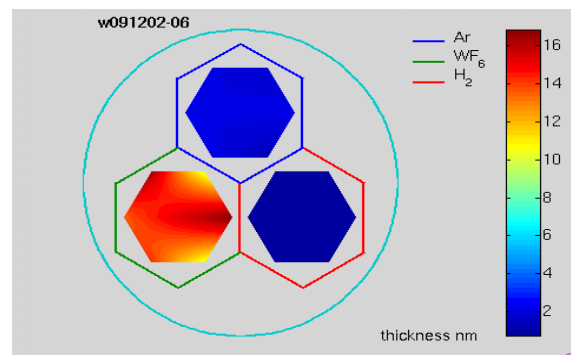


Fig. 6. Deposition thickness profiles corresponding to an experiment in which pure Ar, WF_6 , and H_2 were fed to the individual segments.

3. MODELING AND SIMULATION

Significant effort is being put into developing process simulation tools to assess the effectiveness of the segmented design and to determine the operating conditions for future experiments. Because of the Programmable CVD reactor's reverse-flow design, reactants in the gas mixture in the common exhaust volume can diffuse back into the segments. Therefore, to sustain the pre-specified gas compositions at the bottom of each segment, the back diffusion through the segment should be suppressed below an acceptable level by the convective upward flux contribution.

A steady-state 1-dimensional segment model (for each segment) combined with a well-mixed common exhaust volume model was used to assess the ability of the segmented structure to maintain significant segment-to-segment gas composition differences near the wafer surface. The geometry of a single segment, together with the notation used in the model development, is shown in Fig. 7. A schematic diagram of common exhaust volume is shown in Fig. 8 where each shaded area represents the top of the each segment of the showerhead.

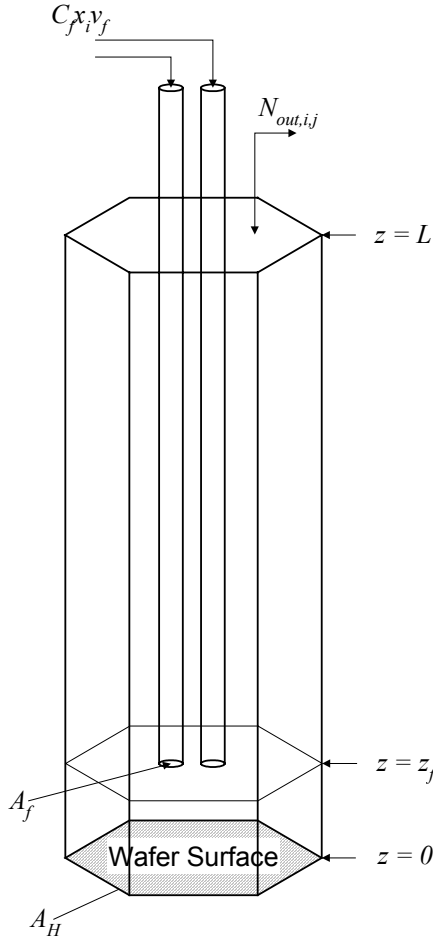


Fig. 7. Schematic diagram of a single showerhead segment.

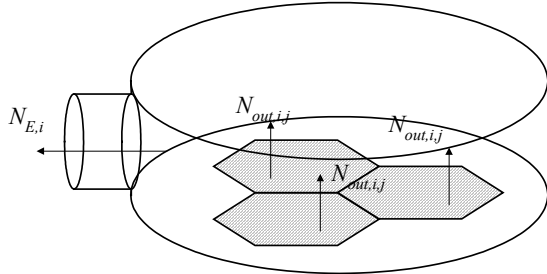
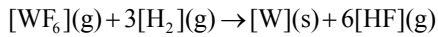


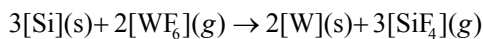
Fig. 8. Schematic diagram of the common exhaust volume.

3.1 Film deposition reactions

The overall reaction of tungsten deposition by hydrogen reduction is



The gas phase reactions associated with this deposition process are negligible due to low reactor pressure during the process operation (Arora and Pollard, 1991; Kleijn *et al.*, 1991). Surface reactions by Si reduction will occur during the film nucleation step



This is a self-limiting reaction and typically accounts for a 10-200 nm of W film thickness (Groenen *et al.*, 1994).

3.2 Multi-component reactant transport.

In the limit of zero distance between the segment wall bottom and wafer surface, the mass balance for each species in each segment can be written as

$$\frac{\partial Cx_i}{\partial t} = -\nabla N_i + F_i, \text{ where } i = 1, 2, \dots, n \quad (2)$$

where C is the total gas concentration in mol/m^3 , N_i is the total flux of species i in $\text{mol}/(\text{m}^2 \text{ s})$, and F_i is a forcing function accounting for the change in flux due to fresh feed of species i from the segment feed tube. At steady-state, (2) can be rewritten as

$$N_i = \begin{cases} \alpha_i R_{\text{kin}} & (0 \leq z \leq z_f) \\ \alpha_i R_{\text{kin}} + C_f x_i v_f \left(\frac{A_f}{A_H} \right) & (z_f \leq z \leq L) \end{cases} \quad (3)$$

where R_{kin} represents the rate of either of the deposition reactions and α_i is the corresponding stoichiometric coefficient of species i in that reaction.

The multicomponent gas species transport can be expressed by the Stefan-Maxwell equation. The binary diffusion coefficient is estimated by the Chapman-Enskog kinetic theory and Neufield method (Kleijn and Werner, 1993; Reid *et al.*, 1987). Neglecting any effect of pressure and forced diffusion, the Stefan-Maxwell equation is written as

$$\nabla x_i = \sum_{j=1, j \neq i} \frac{1}{CD_{ij}} (x_i \bar{N}_j - x_j \bar{N}_i) \quad (4)$$

where

$$\bar{N}_i = N_i + \frac{\mathbf{D}_i^T}{M_i} \nabla \ln T$$

and \mathbf{D}_i^T is the multicomponent thermal diffusion coefficient defined in Kleijn and Werner (1993)

To examine whether back-diffusion of WF_6 from the common exhaust volume through the segments where Ar and H_2 are the only feed gas species can account for the W deposition in these segments, we compute the maximum WF_6 concentration possible for these segments by setting N_i , the total species flux by combined thermal and normal diffusion, to zero at $z=0$ in (3). The boundary condition at the segment top is based on the assumption that the gases leaving each showerhead segment are mixed perfectly in the common exhaust volume (Fig. 8) giving

$$x_{i,j} = \frac{N_{\text{out},i,j}}{\sum_{i=1}^n N_{E,i}} \text{ at } z=L \text{ where } N_{E,i} = \sum_{j=1}^{ns} N_{\text{out},i,j} \quad (5)$$

and where subscript i denotes species number and j refers to segment number. A linear temperature profile was assumed for the gas located in the region

between the wafer and the bottom of the feed gas tube, where it was assumed the gas entered at room temperature.

Given boundary conditions (5), the species moles fractions $x_{i,j}$ can be represented as a function of spatial position by a truncated global trial function expansion. A Galerkin projection method is used to spectrally discretize the system; a Newton-Raphson procedure then is used to solve the resulting set of algebraic equations. For these simulations, it was found that a truncation number of 20 was sufficient to obtain converged solutions to this boundary-value problem.

4. SIMULATION RESULTS

Results of this solution procedure, with simulation conditions set to match the experimental conditions that produced the wafer shown in Fig. 5 are shown in Fig. 9. In this Figure, the wafer surface is located at $z=0$ (the left axis limit) and the segment top is to the right; the vertical line represents the location of the bottom of the feed tube bundle inside each segment.

The top plot shows that for the Segment 1, in which pure Ar is fed, the major gas component is Ar; however, there is significant back-diffusion of H_2 and it appears that sufficient WF_6 diffuses back into the segment to account for the W film found in the experiments. The effect of thermal diffusion is clearly evident in these plots: note how the H_2 profile increases near the heated wafer surface. Similarly, we observe the back-diffusion of WF_6 into the H_2 -fed segment, and the dominance of WF_6 in the segment where only WF_6 is fed. We conclude from this simulation that the potential for significant back diffusion of WF_6 can account for the thin W film deposited in Segments 2 and 3, where no W-containing species were fed.

5. CONCLUSIONS

A novel, spatially controllable CVD reactor design has been developed and a prototype reactor was constructed by modifying a commercial CVD cluster tool. Preliminary simulations and experiments demonstrate the feasibility of producing spatially-patterned film characteristics by controlling gas phase reactant composition directly above the wafer surface

This approach to thin-film manufacturing control opens the door to a new generation of CVD reactor design, allowing single-wafer combinatorial studies and precise across-wafer uniformity control in a single reactor design. Current research focuses on developing a detailed process simulator that will be used to fully exploit the capabilities of this new reactor system.

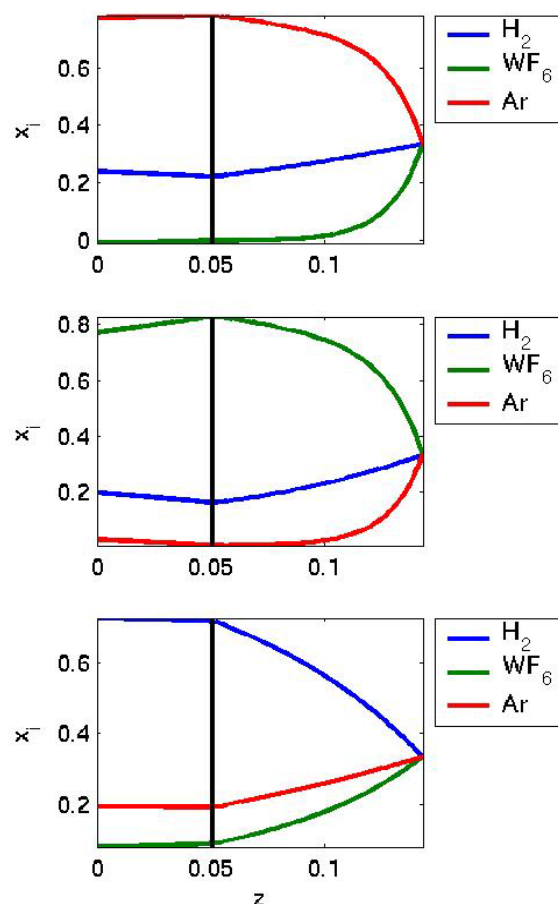


Fig. 9. Reactant gas composition profiles for the 3 segments corresponding pure Ar feed to Seg. 1, WF_6 to Seg. 2, and H_2 to Seg. 3; all at 50sccm.

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