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SDVOSB

# Modeling and Optimization of Film Thickness Variation for Plasma Enhanced Chemical Vapor Deposition Processes

# **OVERVIEW**

This paper describes a method for modeling film thickness variation across the deposition area within plasma enhanced chemical vapor deposition (PECVD) processes. The model enables identification and optimization of film thickness uniformity sensitivities to electrode configuration, temperature deposition system design and gas flow distribution.

PECVD deposition utilizes co-planar 300mm diameter electrodes with separate RF power matching to each electrode. The system has capability to adjust electrode separation and electrode temperature as parameters to optimize uniformity. Vacuum is achieved using dry pumping with real time control of butterfly valve position for active pressure control.

Comparison between theory and experiment is provided for PECVD of diamond-like-carbon (DLC) deposition onto flat and dome geometries. The process utilizes butane reactive feedstock with an argon carrier gas. Radio-frequency plasma is used.

Deposited film thickness sensitivities to electrode geometry, plasma power density, pressure and gas flow distribution are demonstrated. Use of modeling to optimize film thickness uniformity is demonstrated. Results show DLC uniformity of 0.30% over a 200 mm flat zone diameter within overall electrode diameter of 300mm. Thickness uniformity of 0.75% is demonstrated over a 200mm diameter for domed geometry.

Use of the modeling method for PECVD using metal-organic chemical vapor deposition (MOCVD) feedstock is demonstrated, specifically for deposition of silica films using metal-organic tetraethoxy-silane.

Excellent agreement between experimental and theory is demonstrated for conformal and dome geometries.

The model is used to explore scalability of PECVD processes and trade-off against film thickness uniformity.

# 1. INTRODUCTION

Early work by S. W. Ing<sup>1-3</sup> and co-workers, published in the 1960's on low temperature plasma enhanced CVD (or simply PECVD) deposition of silicon oxide films is considered as one of the first experimental reports on the possibility of using electric discharges in gases to produce plasmas that generate different type of reactive species for thin film deposition. These initial attempts were used for microelectronic applications and, in particular, for diffusion masks and passivation. In this regard, the introduction in 1974<sup>4</sup> of commercial batch processing reactors was a definite step in commercial use of plasma-assisted deposition processes in microelectronic circuit production lines.



Low pressure plasma deposition of inorganic films such as silicon-based semiconductors and insulators have gradually moved out of the integrated circuit (IC) industry to new applications in solar cell<sup>5</sup> thin film transistors<sup>6,7</sup> flat-panel displays or micro-electromechanical systems (MEMS)<sup>8</sup> and durable optical coatings such as diamond-like-carbon (DLC and boron phosphide<sup>9,10</sup>.

Use of PECVD for microelectronic applications requires film thickness uniformity control to typically  $\geq \pm 10\%$  over areas up to 300mm diameter. PECVD layers deposited for use in applications such as optical coating<sup>9,10</sup> and solar cells<sup>5</sup> require film thickness control to typically  $\leq \pm 5\%$ . Precision optical coatings may require  $\leq \pm 1\%$  to achieve required spectral location accuracies.

This paper describes a modeling method for film thickness variation within plasma enhanced chemical vapor deposition (PECVD) processes using either conventional reactive gases or metal organic pre-cursor feedstocks. The model enables identification and optimization of deposition process sensitivities to electrode configuration, deposition system design and gas flow distribution. The model specifically quantifies electric field distribution, plasma density, temperature profile and gas flow and relationship with film deposition rate and thickness variation across electrode geometry. The relevant modeled parameters assume radial symmetry inline with deposition system configuration. The flow characteristic, electric potential and temperature distributions are all modeled as each contribute to the process.

Model capability also includes three dimensional substrate structures through import from standard computer aided design packages. Modeling of electric field, gas flow and temperature are included for three dimensional substrate structures. The paper also describes relative contribution of each parameter to overall film thickness variation across both flat and three dimensional parts.

# 2. THE PECVD PROCESS & DEPOSITION SYSTEM

The PECVD deposition system utilized for work reported in this paper is based on a Applied Multilayers LLC designed co-planar 300mm diameter heated electrodes (chamber diameter 600mm) with separate RF (13.56MHz) power matching to each electrode. A diametric view of the PECVD system is shown in Figure 1a.



Figure 1(a) Diametric view of PECVD system configuration.



Figure 1(b) Schematic of PECVD system



Figure 1b shows a schematic diagram of the PECVD system. The heated electrodes can be removed and replaced with alternate electrode size/ geometry. The system has capability to adjust electrode separation (100 to 250mm) and a wide range of other process parameters to optimize uniformity. Accurate control of top and bottom electrode temperature up to 300°C is achievable with an accuracy of  $< \pm 5$  °C over the electrode area.

The system control is fully automatic via a PC/PLC based control system. However, manual control is also available for process development and set-up. Top or bottom electrodes can be separately powered with independent control of plasma bias, process pressure, gas or metal organic feedstock flow and electrode temperature.

Figure 2 shows (a) bottom electrode and (b) top electrodes.



Figure 2(a) Bottom electrode



Figure 2 (b) Chamber with top electrode lifted

The system is also equipped with pumps capable of working with high throughput feedstocks (gas and metal organic feedstocks) and with closed loop process pressure control using a butterfly valve in conjunction with a high accuracy baratron, thereby providing an accurate means to vary the pump speed/ process pressure as shown in Figure 1b.

#### 2.1 Plasma Enhanced Metal Organic Chemical Vapor Deposition

Metal-organic chemical vapor deposition (MOCVD) has been in used for a number of years with tube reactors, and especially for growing dielectric films. However, plasma processing with metal-organics thus far has seen only limited application. The plasma processing configuration using metal organic precursors for the work reported in this paper is shown in Figure 3a: schematic of MOCVD precursor delivery system and b) photograph of MOCVD bubbler assembly..





Figure 3a Schematic of MOCVD precursor delivery system



Figure 3b MOCVD bubbler assembly

The MOCVD precursor delivery system consists of a "bubbler" which allows the organic precursor to be vaporized and become entrained in a stream of argon precursor gas.

Mass flow controller allows precise metering of the carrier gas through the gas train, plus a micron filter and a pneumatic isolation valve. A circular ceramic heater allows uniform heating of the bubbler. Temperature control is via a feedback controller, monitoring a thermocouple in direct thermal contact with the system. The ceramic heater and bubbler are built into a single assembly which can be separated for filling.

Trace heating is provided on incoming (carrier gas only) gas lines and outgoing (carrier gas + precursor) gas lines. This is required to ensure the carrier gas is heated to the correct temperature, and to prevent condensation of precursor in the lines downstream of the bubbler. Gas lead through to allow the precursor gas to enter the chamber and disperse above the top electrode. Due to the thermal mass of the chamber base and the requirement for trace heating, an insulated lead through (normally used for liquid nitrogen transfer) is required.

Pneumatic isolation valve, fitted between the bubbler and the gas lead through, and triggered by the same impulse as the MFC valve.

Prior to operation, the bubbler is filled with the metal organic precursor, and then reassembled (a VCO fitting is built into the bubbler, allowing the two halves to be separated). The samples are then loaded into the chamber, the lid closed, and pumping commences. At the required base pressure, the trace heating and bubbler ceramic heaters are switched on and the temperatures are allowed to stabilize. Deposition commences by opening the bubbler isolation valve, turning on the argon carrier gas, and then igniting the plasma over the substrates. The precursor thus enters the chamber and reacts within the plasma to form deposited material. At the end of deposition the bubbler isolation valve closes, and the carrier gas is switched off.



MOCVD operation is integrated with the control software driving the equipment, with valves and temperature control being asserted automatically. In addition, the MOCVD bubbler is located behind an interlocked panel, inhibiting operation of RF power supplies during load / unload, and the software opens the bubbler isolation valve during venting and initial pump down, to prevent excessive pressure build up.

#### 3.0 MODELING

The key deposition parameters in PECVD are active species partial pressure, temperature, electric field. The deposition rate in a PECVD process can be understood in terms of three steps: - a) chemical activation by electron impact b) transport of active species and c) bonding to film<sup>11,12,13</sup> (Figure 4).



The latter two steps are essentially CVD and governed by the kinetics of the film and gas flow and may be in the kinetic, transport or thermodynamic dominated regimes<sup>14</sup>. A useful way to consider how the deposition rate varies is with gas velocity. The rate increases monotonically to saturation with increasing gas velocity through the three regimes<sup>15</sup>. We take the following as:

$$R/E = \alpha \exp(-\beta/T) (1 - \exp(-\gamma f/(p \text{ vol}_{plasma})))$$

Equation 1

Where  $\alpha$ ,  $\beta$ ,  $\gamma$  are constants of the reaction

T is the substrate temperature f is the flow rate of the precursor gas p is the partial pressure of the unreacted species

E is the electric field (at the surface) vol<sub>plasma</sub> is the volume of the plasma

Here the dependence of the creation rate of precursor (AB) on the plasma volume is included<sup>16</sup>. Using equation 1 and a knowledge of how T, p and [AB] vary the deposition rate over the electrode can be calculated.



## **3.1 Parallel Plate Reactor**

#### 3.1.1 Plasma Potential

It is possible to model the plasma potential by simple finite element methods if we consider the gas in the chamber to be of three materials 1) (un-ionized) gas, 2) plasma and 3) plasma sheath. We consider only the plasma to be a dc current source which results in the self bias at the cathode. The conductivity to this (fictional) dc current is then taken to be a function of the plasma potential for all three materials. In particular it is high at positive potentials and very low for negative ones. Figure 5 shows the potential for a configuration used for DLC in a parallel plate configuration. The potential along a series of vertical lines though the plasma sheath and plasma is shown in Figure 6. These are very similar except at the extreme edge of the electrode. In this planar geometry the field therefore does not introduce non-uniformity over almost all the cathode.







#### 3.1.2 Feedstock partial pressure

Nevertheless there are other factors that can lead to non-uniformity the main one for DLC is the partial pressure of unreacted active component in the feedstock. The source of this is of course the gas fed into the system but there are two sinks namely the system pumping port and also the cathode which pumps the feedstock by converting it into coating. Again finite element methods can be used to model this partial pressure (Figure 7).





## 3.1.3 Temperature

In high durability DLC deposition the heating is from the plasma directly whereas in MOVCD the RF power tends to be much lower and heating is supplied by heaters in the electrodes (Figure 8a). We model the DLC temperature profile by considering a heater layer on the surface, the power in this layer depends on the power in the plasma (Figure 8b).



#### **3.2 Dome geometry**

We now consider a dome to be coated with DLC in the parallel plate reactor.

#### 3.2.1 Plasma potential

In this case the electric field is not necessarily uniform and some care has to be taken to ensure that it is. As above the field can be calculated (Figures 9a and 9b)





This field would be unsatisfactory (too low) at the edge to the extent that there may even be delamination of the DLC. Raising the dome on a platen can increase the field at the edge Figure 10 but in particular example it is too high.



Figure 11 shows the desired condition. Note in this case there also a ring is placed around the dome to remove the discontinuity of the edge of the dome.





# 3.2.2 Temperature

Like the case for the parallel plate geometry the effect of heating by the plasma can be calculated (Figure 12).





# 4.0 RESULTS

#### 4.1 DLC

#### 4.1.1 DLC In Parallel Plate Configuration

The field, partial pressure and temperature profiles can be combined using equation 1 to calculate the deposition rate across the electrode. Figures 13 compare this calculation for three conditions with actual measured rates for these conditions. Note negative and positive grading is predicted and observed for a) and c) respectively. Optimal coating uniform is achieved using condition b)



Figure 13 The measured and calculated deposition rates for DLC in a parallel plate configuration for three deposition conditions. The grading are a) -3.5%, b) +0.3%, c) +2.1% where -ve corresponds to thin in the center.



## 4.1.2 DLC On Dome Configuration

A non-conformal curved geometry based on a 150mm hemispherical geometry was utilized to test modeled performance over a non-planar configuration. Again the three profiles shown in Figure 13 have been modeled with non-conformal geometry and used to calculate the deposition rate. The optimum case is shown in Figure 14 again with very uniform measured values.



Figures 15a and b shows the dome within the deposition system.



(a)

(b)

Figure 15 a) Dome geometry on lower electrode; b) Dummy dome configuration



## 4.2 MOCVD SiO<sub>2</sub>

Essentially the same procedure can be used for MOCVD although as mentioned above the temperature calculation is somewhat different, the constants are also different. Again uniform coatings are achievable over a wide area on the electrode as shown in Figure 16.



#### 5.0 DISCUSSION

A modeling method for film thickness variation within plasma enhanced chemical vapor deposition (PECVD) processes. The model enables identification and optimization of deposition process sensitivities to electrode configuration, deposition system design and gas flow distribution.

The model specifically quantifies electric field distribution, plasma density, temperature profile and gas flow and relationship with film deposition rate and thickness variation across electrode geometry.

Excellent agreement between theory and experiment for reactive gas and MOCVD feedstock is demonstrated. Thickness uniformity  $<\pm1\%$  over 300mm diameter electrode areas have been demonstrated. Such film thickness uniformity levels are required for optical coatings.



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