Analysis of Parameters that Affect Si Layer Properties in a LPCVD Reactor

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Abstract

Low pressure chemical vapor deposition (LPCVD) reactors are used as some of the most prominent equipment to use in microelectronic industries. In this report, a LPCVD reactor is modeled as a 3-zone boat reactor to determine both the deposition rate of silicon and the uniformity of the wafer using various parameters. The parameters that were tested were the spacing of the wafers, total pressure of the boat reactor, and the inlet mole fractions of silane, SiH_4, and hydrogen, H_2. The results were analyzed using an interaction chart and a Pareto diagram, which concludes that the spacing of the wafers and mole fractions of SiH_4 represented the most impactful parameters out of the ones chosen. Some considerations to implement for future experiments dealing with LPCVD reactors include having more parameters to test on the boat reactor. Overall, the results represent how there are multiple parameters to account for the impact on the deposition rate of silicon, Si, and the uniformity of the wafer.

1 Introduction

Since the 1980s, LPCVD is used as a thin film deposition technique to perform micromachining processes.[1] The use of thin film depositions are used throughout modern technology. These film depositions are considered to create these small molecule layers that are applied to various kinds of substrate materials throughout the reactors. Materials such as glass, silicon, and many others are altered to help understand what specifically changed with the substrates, whether it would change its physical properties or even enhance the material itself. Two important deposition techniques are called physical vapor deposition (PVD) and chemical vapor deposition (CVD). PVD is the use of various methods that generate a flow of materials into a form of coating, whereas CVD uses a form of organometallic compound that is used to transform the compound into vapor state and perform deposition, which is where coating occurs.[2] Comparing both techniques, both use the concept of film deposition. PVD and CVD have their advantages and disadvantages. A disadvantage to account for CVD is that CVD is required to operate at higher parameters compared to PVD.[2] Parameters such as temperature and pressure are needed in order to provide high efficiency coming from CVD.[2] Compared to PVD, the technique itself is only funneled by using low pressure and temperature.[3] An advantage for CVD is the adjustment of synthesis with pressure. With the process of synthesizing lower pressures with a higher pressure phase, excitement can occur, which allows more room to increase the rate of deposition just by using the thermodynamic conditions of the given compounds.[3] These deposition techniques overall are used in companies like microelectronic industries, where manufacturers would use technology like LPCVD to create nanofabrication.[4] Using LPCVD reactors are beneficial in industry since they can improve on designs of materials, flexibility in different chemistry bounds being used, and much more.[4] Overall, LPCVD has its advantages compared to other modern technology being used today.

2 Background

LPCVD reactors have many advantages compared to other options due to its mechanism. LPCVD works by flowing precursor gases through a low pressure chamber where it passes by heated substrates.[5] Deposition begins to form on the substrates due to chemical reactions.[5] By-products and unreacted precursor gases are then vented out of the chamber.[5] The mechanism of LPCVD allows it to excel in uniformity, purity, and reproducibility compared to other methods.[6] Although this seems like a straight forward process, LPCVD is a complicated process due to the variety of parameters that can change the deposition rate and uniformity, especially depending on the setup.

Parameters such as temperature is one of the most significant, if not the most significant parameter that affect LPCVD.[7] Since, LPCVD is dependent on chemical reactions, temperature would increase the rate of reaction leading to an increase in deposition rate while still having good uniformity.[7] However, other parameters such as inlet mole fraction and wafer spacing may not be as evident.

In this report, we show how parameters such as inlet mole fraction of H_2 and SiH_4, pressure, and wafer spacing independently and in combination affect Si deposition rates and uniformity for LPCVD of a 3-zone boat reactor in COMSOL.

3 Theory

The three-zone boat reactor is called a three-zone reactor because there are three distinct zones where temperature is independently controlled by a heater. The first zone is the pre-heating zone, the second zone is the wafer zone, and the third zone is the downstream zone.[8] The three-zone boat reactor is separated into two regions. Region 1 is the boat reactor, while region 2 is the actual wafers. To model the 3-zone boat reactor in COMSOL, as seen in Figure 1, multiple equations and boundary conditions were used to simulate the wafer and reactor region.

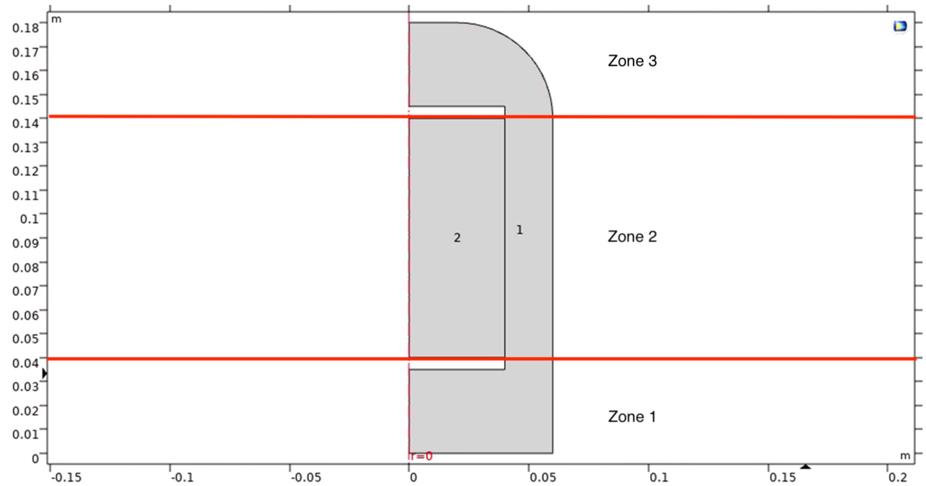

Figure 1: This figure shows the three-zone boat reactor used for the simulation in COMSOL

The reaction occurring in the LPCVD reactor is listed below.

$$SiH_4\,(g) \longrightarrow Si\,(s) + 2\,H_2\,(g) \tag{1}$$

There are many physical phenomena that play a role in this reaction. For instance, the way the reactants flow determines the extent of reaction. Thus, to simulate fluid dynamics for the boat reactor region, the Navier-Stokes equation was used

$$\rho(u \cdot \nabla)u = \nabla \cdot [-pI + K] + F \tag{2}$$

where ρ is fluid density, u is the velocity of the fluid, p is the pressure, I is the unit directional vector, F is the external forces on the fluid, and K is

$$K = \mu(\nabla u + (\nabla u)^T) \tag{3}$$

where μ is the fluid's dynamic viscosity, and T is the temperature. Also,

$$\rho\nabla \cdot u = 0 \tag{4}$$

with the same variables being defined just above. It is important to note that the fluid was considered incompressible and fully laminar.

Another important aspect for the extent of the reaction is the mass transfer of the reactants onto the substrate. Therefore, to simulate the convective mass transfer for the reactor and wafer region, Fick's Law of Diffusion was used

$$\nabla \cdot J_j + u \cdot \nabla c_j = R_j \tag{5}$$

where J_j is the molar flux of species j, c_j is the concentration of species j, and R_j is the rate of reaction for species j. Also, J_j is defined as

$$J_j = -D_j \nabla c_j \tag{6}$$

where D_j is the diffusion coefficient of species.

Lastly, heat transfer is important to the extent of reaction as temperature plays an integral part in the rate of reaction. Thus, in order to simulate heat transfer in the reactor and wafer region, Fourier's Law was used

$$\rho C_p u \cdot \nabla T + \nabla \cdot q = Q + Q_p + Q_{vd} \tag{7}$$

where C_p is the heat capacity, q is the heat flux, Q is the heat source, Q_p is the pressure work, and Q_{vd} is the viscous dissipation, and q is defined as

$$q = -k \nabla T \tag{8}$$

where k is the thermal conductivity.

COMSOL uses these governing equations alongside the boundary conditions in Table 1 to solve these equations simultaneously to calculate silicon deposition rate. The silicon deposition rate as well as the effectiveness factor is are important metrics that quantify how well the

LPCVD works. Deposition rate of silicon is an important metric for throughput, as it determines how fast the silicon can grow to the desired thickness. The effectiveness factor is

$$\eta = \frac{\Delta_{\mathrm{Si}}^{avg}}{\Delta_{\mathrm{Si}}^{edge}} \tag{9}$$

where $\Delta_{\mathrm{Si}}^{avg}$ is the average deposition rate of silicon on the wafer and $\Delta_{\mathrm{Si}}^{edge}$ is the silicon deposition rate on the outer edge of the wafer. The effectiveness factor is important as it defines how uniform the silicon layer is on the wafer and thus its quality.

Table 1: Boundary conditions for the COMSOL simulation and their respective explanations.

Boundary Condition	Explanation
Fluid Dynamics	
$u_{r=0} = u_{z=0} = 0$	Velocity at inlet in r and z direction is 0 m/s
Mass Transfer	
$c_{\mathrm{Si}_4} = c_{10}$	Initial concentration of SiH_4 is c_{10} mol/m^3
$c_{\mathrm{H}_2} = c_{20}$	Initial concentration of H_2 is c_{20} mol/m^3
Heat Transfer	
$T_j = T_0$	Initial temperature in region j is T_0

4 Methods

Throughout this experiment, an LPCVD reactor was modeled as a 3-zone boat reactor in COMSOL to determine which parameters would affect silicon layer properties.[9] The parameters that were chosen to vary were the wafer spacing, d_{cc}, total pressure, p_{tot}, and inlet mole fractions of silane and hydrogen, y_{0,SiH_4} and y_{0,H_2}. The main point of choosing these parameters was to determine which ones would affect both the deposition rate of silicon, ΔSi, and the effectiveness factor, eta. Changing the wafer spacing would allow for more reactants to flow in and interact with the substrate. Total pressure was chosen as a parameter in order to understand how an increase or decrease of pressure would affect the deposition rate of silicon since the simulation was initially running at low pressure. The inlet mole fractions of silane and hydrogen were used as parameters to understand the chemical reaction occurring throughout the simulation. Specifically, this helps determine how both the inlet mole fractions affect the deposition rate of silicon since the amount that can be grown on the surface depends on the availability of the reactants. All of these parameters varied around ±5% of the initial values stated within the LPCVD simulation, and COMSOL reported at most 16 different combinations. The purpose of varying around 5% was to keep it as close to the initial parameters given in the boat reactor but still collect data that might be significantly different. The data is both graphed and plotted out using an interaction chart and a Pareto chart. Interaction charts help display information on the high and low variations of the parameters, whereas the Pareto chart displays the parameters with the biggest impact for both deposition rate of silicon and the effectiveness factor using the slopes that were calculated using the information from the Pareto charts.

5 Results and Discussion

The experimental data from the LPCVD simulation was collected and used to create interaction plots that demonstrated the effect of high and low variation of each parameter on the average η and Si deposition rate. The Pareto charts ascertained from the data demonstrated the extent of the effects the parameters had on the Si deposition rate and average η.

Figure 2 demonstrates how significant the effects are from each of the parameters on average η. A steeper line would indicate that the change in that parameter would result in a significant change in the average η. Looking at Figure 2 and Figure 3, the figures show the extent of the effect for each of the parameters on average η. Figure 3 shows that wafer spacing, d_{cc} and the inlet mole fraction of SiH_4, y_{0,SiH_4}, have the largest positive contribution to average η. Figure 3 also shows the interaction between the wafer spacing and the inlet mole fraction of SiH_4 which shows a negative contribution to the η. Other parameters such as total pressure, p_{tot}, the interaction between p_{tot} and d_{cc} had a smaller contribution to η. Every other parameter and interaction between the parameters such as y_{0,H_2}, p_{tot} and y_{0,H_2}, p_{tot} and y_{0,H_2}, y_{0,SiH_4}

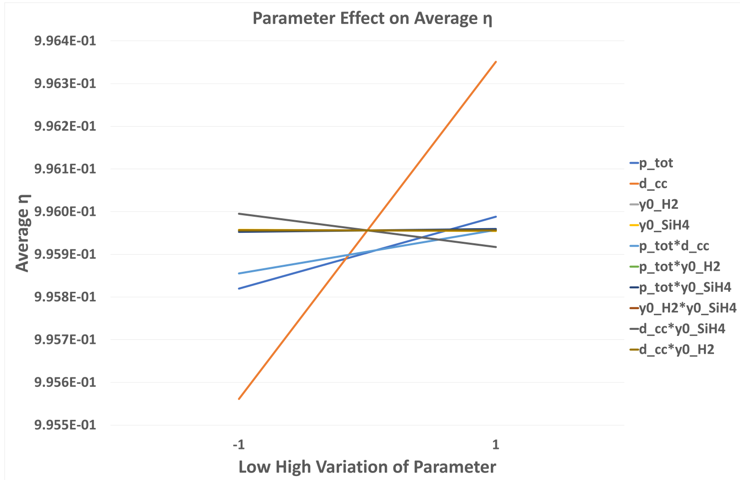

Figure 2: The figure demonstrates how high and low values of each parameter affect average η.

and y_{0,H_2}, and d_{cc} and y_{0,H_2} had little to no contribution to the average η of each wafer.

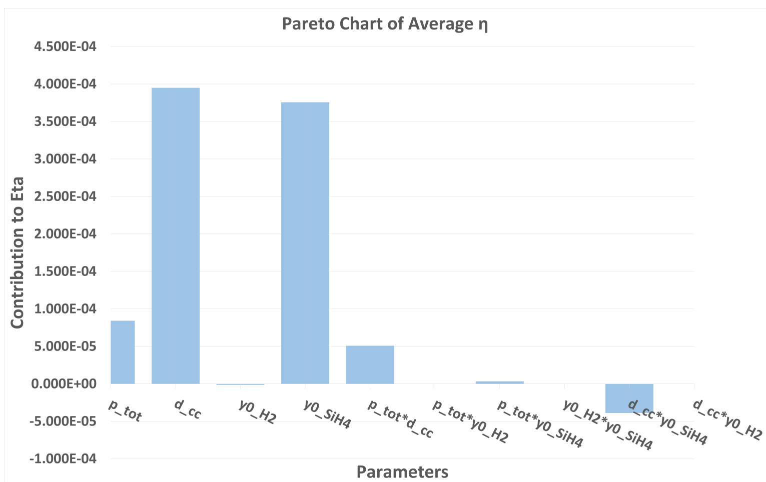

Figure 3: This figure shows the extent of the contribution each parameter has on the average η.

The results of Figure 2 and Figure 3 show that y_{0,SiH_4} and d_{cc} had the most significant effect on the average η. These results are to be expected because a large d_{cc} allows for SiH_4 to be more effectively evenly dispersed onto the wafer which causes the average η to be affected more significantly by the wafer spacing, d_{cc}. With regards to y_{0,SiH_4}, the result is also to be expected because SiH_4 will affect the silicon deposition rate which would affect the average η because η is a function of the silicon deposition rate. With regards to the other parameters, such as total pressure, it is shown to make some contribution to η, but the total pressure contribution is expected to be small because the total pressure will only affects the uniformity of the silicon deposition.[5]

Figure 4: The figure demonstrates how high and low values of each parameter effect the Si deposition.

Looking at Figure 4, the interaction chart shows how a change in a parameter may change the silicon deposition rate. In conjunction with Figure 5, the extent of the effect for each of the parameters on the silicon deposition rate can be observed quantitatively and qualitatively. From Figure 5, it is apparent that $y_{0,\mathrm{SiH_4}}$ is the parameter that most significantly contributed to the change in the silicon deposition rate. The two other parameters that also made a measurable contribution to the change in the silicon deposition rate were p_{tot} and d_{cc}. All other parameters made little to no significant contribution to the change in the silicon deposition rate.

The results shown by Figure 4 and Figure 5 show that a change in $y_{0,\mathrm{SiH_4}}$ contributes to a significant change to the silicon deposition rate and that by increasing $y_{0,\mathrm{SiH_4}}$ there is a positive contribution to the silicon deposition rate. An increase in $y_{0,\mathrm{SiH_4}}$ increases the amount of silicon present when the reactions occur; therefore, the silicon deposition rate should increases. As a result, the findings from Figure 4 and Figure 5 are to be expected. With regards to p_{tot}, the positive contribution from p_{tot} is also expected because the p_{tot} parameter enables the control

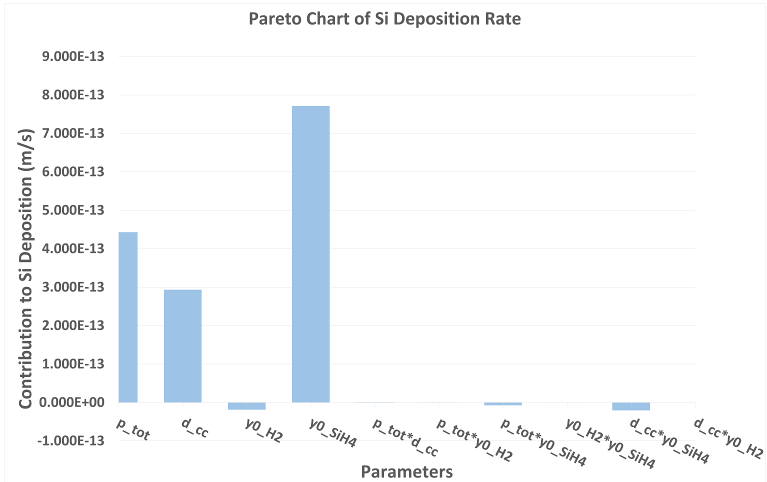

Figure 5: This figure shows the extent of the contribution each parameter has on the deposition rate of Si.

of the uniformity of the silicon wafers thereby controlling the silicon deposition rate.[5] In terms of d_{cc}, the positive contribution is also expected because a larger wafer spacing would allow for more SiH_4 to flow over the wafer, therefore increasing the silicon deposition rate. As a result, $y_{0,\mathrm{SiH_4}}$ and d_{cc} had the most measurable effect on η, comparatively, whereas $y_{0,\mathrm{SiH_4}}$, p_{tot} and d_{cc} had a measurable effect on the silicon deposition rate compared to the other parameters.

6 Conclusions

In conclusion, the parameters chosen for the 3-zone boat reactor in COMSOL were compared and analyzed with each other. Based on the Pareto chart, there is a visualized representation in which both d_{cc} and $y_{0,\mathrm{SiH_4}}$ impacted η the most. As for the ΔSi, d_{cc} and $y_{0,\mathrm{SiH_4}}$ are represented on its respective Pareto chart as the most impacted parameters out of the rest of 4 parameters tested. This would be expected for $y_{0,\mathrm{SiH_4}}$ since changing the amount of silane present at the inlet would change how much can be deposited on the solid, resulting in $y_{0,\mathrm{SiH_4}}$ having a large contribution to both η and ΔSi. As for d_{cc}, this was also to be expected since the amount of spacing affects how much reactant can react with the substrate in the wafer region of the 3-zone boat reactor. Thus, the parameter is a large contributor to η and ΔSi. Some considerations in order to improve the lab involve testing more parameters. By increasing the amount of parameters, more data can be retrieved and analyzed to see what other parameters impact the simulation.

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(9) COMSOL Boat reactor title `www.comsol.com` (accessed 05/25/2022).

Appendix

1. Solution-Based Photo-Patterned Gold Film Formation on Silicon Nitride
    - Author(s): Bandara, Y. M.; Karawdeniya, B. I.; Whelan, J. C.; Ginsberg, L. D.; Dwyer, J. R.
    - Year published:2016
    - Journal name: ACS Applied Materials & Interfaces
    - 1-3 major accomplishments of this paper:
        (a) Uses LDCVD for modern industries, in this case, to create nanofabrications
        (b) Created a spatially pattern, which develops more leverage and benefits for thin films.
2. Development of the Modern Vacuum Coating Technologies
    - Author(s): Vasin, V. A.; Krit, B. L.; Somov, O. V.; Sorokin, V. A.; Frantskevich, V. P.; Epel’fel’d, A. V.
    - Year published: 2016
    - Journal name: Surface Engineering and Applied Electrochemistry
    - 1-3 major accomplishments of this paper:
        (a) Found the differences of the deposition techniques between physical and chemical vapor deposition
3. Development of Diamond Synthesis Techniques at Low Pressures
    - Author(s): Matsumoto, S.
    - Year published: 2000
    - Journal name: Thin Solid Films
    - 1-3 major accomplishments of this paper:

    (a) Various diamond synthesis techniques were created using various CVD methods
    (b) Modern technology, such as laser and microwave discharge, are implemented with the CVD methods that are based on Matsumoto's research

4. Low-Temperature LPCVD MEMS Technologies
    - Author(s): Howe, R.; King T.
    - Year published: 2002
    - Journal name: Mat. Res. Soc. Symp. Proc.
    - 1-3 major accomplishments of this paper:
        (a) Use of LPCVD processes for fabrication
        (b) Research and development of poly-SiGe technology for future processors

5. Development of an integrated physical vapour deposition and chemical vapour deposition system
    - Author(s): Mundra, S.S.; Pardeshi, S.S.; Bhavikatti, S.S.; Nagras, A.
    - Year published: 2021
    - Journal name: Materials Today: Proceedings
    - 1-3 major accomplishments of this paper:
        (a) Explanation of how PVD and CVD work.
        (b) Shows how certain parameters effect extent of reaction.

6. A Mathematical Model of the Hydrodynamics and Gas-Phase Reactions in Silicon LPCVD in a Single-Wafer Reactor
    - Author(s): Kleijn, C.R.
    - Year published: 1991

- Journal name: Journal of the Electrochemical Society
- 1-3 major accomplishments of this paper:
  (a) Explains why CVD is preferred over other methods.
  (b) Shows how certain parameters such as pressure and temperature affect silicon growth rate.

7. Analysis of Multicomponent LPCVD Processes: Deposition of Pure and In Situ Doped Poly-Si
   - Author(s): Roenigk, K.F.; Jensen, K.F.
   - Year published: 1985
   - Journal name: Journal of the Electrochemical Society
   - 1-3 major accomplishments of this paper:
     (a) Describes reaction mechanisms involved in silicon growth on wafers.
     (b) Shows how certain parameters such as pressure and temperature affect silicon growth rate.