Simulation of reactor and design of thermal insulation structure for vertical furnace

Shuai Yang¹, Jiannong Song¹,²* and Nan Sun¹
¹College of Engineering, China Agricultural University, Beijing, China
*Corresponding author e-mail: songjn@cau.edu.cn

Abstract. The temperature and airflow distribution of the reactor are the important factors that influence the thickness uniformity of the silicon film. In this paper, the vertical furnace reactor is studied by finite element simulation, and the thermal insulation structure is designed and tested. The influence of the temperature distribution of the silicon wafers on the bottom of the reactor is studied by changing the parameters of the thermal insulation structure. The results show that the change of the number, diameter and the material of the thermal insulation sheets have significant influence on the uniformity of the temperature of the silicon wafers. According to the thermal insulation structure determined by the experiment, the uniformity of the film thickness is guaranteed, which provides important data support for the design of the reactor.

1. Introduction
Chemical vapor deposition is an important process method for chip manufacturing. The effect of heat radiation on the heat transfer under low pressure is significant⁴, and the effect of gas convection on the temperature field is much smaller than that of the atmospheric pressure environment⁵. The film thickness uniformity is an important evaluation index for the film forming quality of silicon wafer. The temperature distribution on the surface of silicon wafer directly affects the thickness of the chemical vapor deposition film⁶. Therefore, it is of great significance to study the temperature field distribution characteristics and the adjustment method of the reactor, which is of great importance to the design of the chamber structure. It is also of great significance to study airflow field distribution of the reactor.

The distribution of temperature field and airflow field in the reactor determines the uniformity of silicon film thickness directly. For the 300mm vertical furnace reactor, the method of combining simulation and experiment is used to study the distribution characteristics of the temperature field and the airflow field in the chamber. The influence of different parameters on the thickness of silicon wafers was analyzed by means of the design of different thermal insulation structures to control the surface temperature of silicon wafers.

2. Simulation modeling of reactor
The reactor is mainly composed of process tube, boat, thermal insulation structure, thermocouple, heater and Manifold, as shown in Figure 1. The reactor, through the process tube, causes the heat treated silicon to be isolated from the outside to form a sealed chamber. The process tube is a double layer tube, which is divided into inner tube and outer tube. The inner tube is a place for the reaction of silicon wafer. The vacuuming between the inner tube and the outer tube causes the reaction chamber
to form a low pressure environment. The process tube should be able to accommodate a boat and a
thermos barrel. A boat can carry multiple silicon wafers. The thermal insulation structure is used to
maintain the constant temperature of the reaction chamber. Meanwhile, the parts under the thermal
insulation structure are protected by the high temperature of the chamber. The process gas enters the
reaction chamber from the Manifold and is discharged from the exhaust port after the reaction. The
thermocouple is used to control the temperature in the chamber of the reactor.

Figure 1. Structure diagram of reaction chamber.

1- process tube; 2- boat; 3- thermal insulation structure; 4- manifold; 5- thermocouple; 6-heater

The reaction chamber is the heat treatment place of silicon. The material of the reaction chamber is
required to tolerate high temperatures above 1000 °C. The metal and other pollutants can not be
precipitated at high temperature. The material is optional SiC or quartz, but the cost of SiC is higher.
SiC is more brittle and easy to break. In order to reduce the cost, quartz material is preferred. Content
of impurities in several common quartz materials is shown in table 1. GE214 can be used as a
processing material according to the requirement and cost of the equipment process index.

Table 1. Content of impurities in several common quartz materials (ppm by weight).

| Grade | Al | Ca | Cu | Fe | Li | Mg | Mn | K | Na | Ti | Zr | OH content |
|-------|----|----|----|----|----|----|----|---|----|----|----|----------|
| GE214 | 14 | 0.4| <0.05| 0.2| 0.6| 0.1| <0.05| 0.6| 0.7| 1.1| 0.8| 10       |
| GE224 | 14 | 0.4| <0.01| 0.2| 0.001| 0.1| <0.05| 0.2| <0.1| 1.1| 0.8| 10       |
| GE244 | 8  | 0.6| <0.03| 0.2| <0.2| <0.1| <0.03| 0.2| <0.2| 1.4| 0.3| 10       |

The reaction chamber is simulated by the finite element software Ansys. According to the
simulation results, the distribution of the temperature field and the airflow field in the chamber are
studied. The simulation conditions are set up according to the requirements of the process. The
pressure of the reaction chamber is 34pa. Inlet pressure is 300kPa. The temperature of the heater is
780°C. NH3 is 2000sccm. SiCl2H2 is 200sccm.

3. Analysis of simulation results
The distribution of flow field in the process tube is determined by simulation, especially the
uniformity of SiCl2H2 and NH3 in the films. After the simulation, the cross section of the wafer
surface is established on the 1, 31, 62 and 125 pieces. The distribution of SiCl2H2 mass fraction, NH3
mass fraction, pressure and velocity on several sections is analyzed. It gets worse from the top down between the outer tube and the inner tube.

Figure 2. Distribution of mass fraction of SiCl₂H₂ and NH₃.

As shown in figure 2, the distribution of SiCl₂H₂ mass fraction is known from a. It gets worse from the top down between the outer tube and the inner tube. In the inner tube area, the distribution of SiCl₂H₂ mass fraction is more uniform. The distribution of NH₃ mass fraction is known from b. It gets worse from the top down between the outer tube and the inner tube. Inside the inner tube, the distribution of NH₃ mass fraction is more uniform. Therefore, the reaction area of the silicon chip is even better inside the inner tube, which is beneficial to the uniform chemical reaction of the process gas on the wafer.

Figure 3. Pressure and velocity distribution of fluid.

As shown in Figure 3, the pressure distribution of the chamber is known from a. The maximum pressure difference at the bottom is 100kpa, and the top pressure difference is 3pa. The pressure difference increases gradually from the top to the bottom of the inner tube, which is mainly due to the pressure fluctuation of the 300kpa process gas entering the reaction chamber from the bottom. The pressure fluctuation decreases as the gas enters the upper chamber. The pressure difference between the outer tube and the inner tube is small, and the vacuum degree is significantly higher than the inner tube. This is mainly due to the negative pressure of the exhaust pipe line between the outer tube and the inner tube. As a result, the thickness uniformity of the silicon film at the bottom of the reaction chamber is greatly influenced by the pressure, which is not conducive to the uniformity of the film thickness. It is known from b the velocity distribution of the fluid. The maximum speed is 10m/s at the bottom. The maximum speed of the rest is 8m/s. The speed is fast at both ends of the chamber, which is mainly due to the rapid impact of the flow on the fluid at the bottom. At the top, the overall speed is suddenly faster because that the top is not shielded to facilitate the rapid flow of the fluid. The single silicon wafer gradually increased in a circular ring from the center to the edge. This is mainly because that the gap between the silicon wafers is 7mm far less than the gap between the silicon wafers and the inner tube. Gas is more likely to pass through the gap between the silicon wafers and the inner tube so that the velocity of the edge of the silicon wafer is faster than that at the center. The velocity difference between the outer tube and the inner tube is little, and the speed is faster than the inside of the inner
tube, which is mainly due to the larger pumping speed of the exhaust pipe. As a result, the thickness uniformity of the membrane at both ends of the reaction chamber is greatly influenced by the velocity of the fluid, which is not conducive to the uniformity of the film thickness.

To sum up, the simulation results show that the thickness uniformity of the silicon film in the middle of the reaction chamber is better than that of the two ends. The bottom is influenced greatly by the pressure difference, and the top is influenced by the velocity difference. For a single silicon wafer, the pressure at the edge is greater than that of the center, and the velocity of the fluid at the edge is greater than that of the center. The edge of the silicon film is slightly thicker than that of the center.

4. Experiment

Figure 4. Measuring temperature with TC-Wafer.

In this experiment, a new LPCVD device is used to test it. In the experiment, the temperature of the heater is 800℃, and the chamber pressure is 34pa. As the thermal insulation structure has a great influence on the bottom temperature of the reactor, several groups of thermal insulation are designed for testing. The analysis shows that the temperature distribution at the bottom of the reaction chamber is mainly influenced by the thermal insulation sheets on the top of the thermal insulation structure. In the experiment, the temperature distribution of the silicon wafer was measured by TC-Wafer, as shown in Figure 4.

Table 2. Temperature test of different thermal insulation sheets.

| Test | Material | Quantity | Diameter /mm | Range/℃ |
|------|----------|----------|--------------|---------|
| 1    | OP3      | 4        | 248          | 1.6     |
| 2    | OP3      | 8        | 248          | 1.2     |
| 3    | SiC      | 4        | 248          | 4.2     |
| 4    | OP3      | 16       | 248          | 1.7     |
| 5    | OP3      | 16       | 150          | 1.9     |

The temperature distribution of the eighth slices of silicon at the bottom in combination with different thermal insulation sheets is shown in Table 2. Range indicates the difference in surface temperature, which is the difference between the average value of the edge temperature and the average temperature of the center. It can be seen from Test1 and 2 that the number of SiO₂ thermal insulation sheets with a diameter of 248mm is increased at the top of the thermal insulation structure, the Range decreases, and the temperature uniformity in the bottom silicon wafer is better. The heat capacity of SiO₂ is less than SiC. It is known by Test1 and 3 that the material of thermal insulation sheets is changed from SiO₂ to SiC, and the Range becomes larger. The temperature uniformity in the
surface of the bottom silicon wafer is worse. It is known from Test4 and 5 that the diameter 248mm of the thermal insulation sheet becomes 150mm, and the Range becomes larger. The temperature uniformity in the surface of the bottom silicon wafer is worse.

To sum up, increasing the number of the top thermal insulation sheets is conducive to the uniformity of the temperature of the bottom silicon wafers. If the diameter of the thermal insulation sheets is properly increased, the temperature uniformity of the bottom silicon wafers is good. The thermal insulation sheets made of quartz is beneficial to the temperature uniformity in the surface of the silicon wafer. Therefore, the process test is carried out according to the data selection of 8 quartz thermal insulation sheets with a diameter of 248mm.

![Figure 5. Thickness distribution map of silicon film.](image)

The LPCVD process was used to produce a film on the surface of the silicon wafer. The thickness of the film was measured at each position after the process was completed. Figure 5 shows the thickness distribution of silicon film. And a shows the thickness distribution map of the top silicon film, b shows the thickness distribution map of the central silicon film, and c shows the thickness distribution map of the bottom silicon film. The film thickness at the center of a, b and c is thinner than that of the edge, which is in accordance with the simulation results. The STD of a is 6.56 Å. The STD of b is 6.11 Å. The STD of c is 6.89 Å. This index is less than 10 Å, which meets the process requirements. The three membrane thickness mutation points on the silicon wafer are related to the structure of boat. The contact area between the boat and the silicon wafer needs to be reduced. The effect of the boat on the thickness of silicon film is reduced. The uniformity of film thickness is improved. It provides important experimental data for the optimization of the structure of the boat.

![Figure 6. Thickness distribution of silicon film at the bottom of the reaction chamber](image)

As shown in Figure 6, the thickness of the 49 points of the silicon wafer at the bottom is measured. This is used to verify the effect of improving the thickness uniformity of the film after optimizing the thermal insulation structure. Compared with the data of the baseline platform, the thickness distribution of the film is basically consistent with the data of the baseline machine. This shows that the thermal insulation structure basically meets the requirements of the process. However, the number of mutations at the 33 point is greater than that of the baseline machine. This is a point of contact with the silicon wafer and the boat. It is necessary to optimize the structure of the boat. Therefore, it is
proved that the thickness of silicon film at the bottom of the reactor is significantly affected by the temperature distribution.

5. Conclusion

Through the combination of modeling simulation and experimental optimization design, a vertical furnace reaction chamber for LPCVD process is designed in this paper. Silicon wafer can be processed in batch. Several important factors that affect the process result are analyzed by simulation. Then, the process verification is carried out. The thickness distribution of silicon film in three positions of the reactor is analyzed, and all of them meet the requirements of the process. The thickness uniformity of the silicon film at the bottom of the reaction chamber is greatly influenced by the thermal insulation structure. By changing the three influencing factors of the number, material and diameter of the thermal insulation sheets, the silicon wafer temperature test at the bottom of the reaction chamber is carried out, and the optimal thermal insulation structure scheme is obtained. It can be seen from the process results that the uniformity of the film thickness is basically satisfied. Therefore, the thickness uniformity of the silicon film treated by this vertical furnace chamber can satisfy the growth of CVD film and prepare high quality silicon wafer.

Acknowledgments

The authors would like to acknowledge the supports received from the National Key Research and Development Plan (2016YFD0701605/2016YFD0700302).

References

[1] Michael Quirk, Julian Serda. Semiconductor Manufacturing Technology. Prentice Hall, 2000, pp. 24-34.

[2] Yang Wang, Liu Xueping, Xia Huanxiong, et all. Simulation of Temperature Profile and Design of Heat Transfer Structure for Reactor of film Growth on Si-Wafer. vacuum science and technology, 2016, 36(01):103-109(in Chinese).

[3] Duan Wenrui, Tian Ling, Wu Yuanhao, et all. Design Optimization of Confinement Ring in Reactive Ion Etching Reactor of 450 mm Silicon Wafer. vacuum science and technology, 2015, 35(01):89-99(in Chinese).