Simulation and Optimization of Temperature Field in Large-Sized MOCVD Reactor by Resistance Heating

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Abstract. The effect of the number of layers and the length of the heat shields on the heating efficiency and temperature distributions in the substrate have been studied by establishing the model of a single-piece 18-inch MOCVD reactor. The results show that the number of layers of the heat shields is directly proportional to the heating efficiency, decreasing the length of the thermal shield can reduce the standard deviation (STD) of the substrate temperature. When the length of the heat shields is 56mm, the coefficient of substrate temperature STD is 21.41°C and the STD is about 45% lower than the traditional susceptor. An area within substrate radius of 200mm, the coefficient of substrate temperature STD is 2.64°C and the STD is about 93% lower than the traditional susceptor. The results obtained will provide theoretical basis for developing the heating structure of large-sized MOCVD reactor.

1. Introduction
MOCVD is an abbreviation for Metal-organic chemical vapor deposition and is an important technology for preparing nitride semiconductor materials[1-2]. With the maturity of the third generation semiconductor technology, the market demand for semiconductor devices is increasing, and the quality of semiconductor thin film materials is becoming more and more demanding[3]. Due to the complexity of MOCVD technology, the film growth process is affected by many factors [4-8], among which the uniformity of substrate temperature distribution is an important factor affecting the growth of the film[9-14]. However, in the conventional resistive heating system, the heating efficiency and temperature uniformity of large-sized substrate are more prominent. In this work, the influence of the number of layers and the length of the heat shields on the heating efficiency and the uniformity of substrate temperature distribution have been studied by establishing an 18-inch MOCVD reactor model of resistance heating, aimed at improving the heating efficiency of the heating system and the uniformity of substrate temperature distribution.
2. Model of MOCVD Reactor

The growth mechanism of MOCVD is complex and affected by many parameters. Usually, the finite element method is used to establish a mathematical model, and the thermal field and the fluid field are coupled and calculated. The mathematical model uses the fluid equation and heat conduction equation of STR's VR-Nitride simulation software.

Heat conduction equation:

\[ \rho C_p \frac{\partial T}{\partial t} + \nabla \cdot (-k \nabla T) = Q - \rho C_p \nabla T \]  

(1)

Fluid equation:

\[ \rho \frac{\partial \vec{u}}{\partial t} - \eta \left( \nabla \vec{u} + (\nabla \vec{u})^T \right) + \rho \vec{u} \cdot \nabla \vec{u} + \nabla p = 0 \]  

(2)

Where \( \rho \) is density, \( C_p \) is specific heat, \( T \) is temperature, \( k \) is material thermal conductivity, \( Q \) is resistance heating, \( \vec{u} \) is gas velocity, \( \eta \) is gas viscosity coefficient, and \( p \) is pressure. In order to improve the calculation speed in the simulation experiment, the following assumptions are made for the model without affecting the main simulation results:

1. Neglect of the chemical reaction between gases;
2. Assume that the gas is ideal gas;
3. The wall temperature of the reaction chamber is constant;
4. The thermal expansion of the materials is not considered.

![Figure 1. Geometrical model of MOCVD reactor](image_url)

Figure 1. shows a schematic diagram of a two-dimensional axisymmetric structure of the MOCVD reactor, including the wall, an inlet and an outlet, heating resistors, a substrate, and heat shields. The susceptor material is graphite, and the heating resistors under the susceptor and the components of the heat shields are tungsten and molybdenum, and the number of layers of the heat shields can be set to 0 or more. The simulation model susceptor height \( H \) is 19.05mm, the substrate radius \( R \) is 232.6mm, and the number of the heating resistors is 5, and the resistance power density is 7.5E+007W/m³. The distance between the adjacent heating resistors is 4mm. The length of the heat shield is 148.7mm and the width is 2mm, and the interval between the heat shields is 2mm.

In the simulation process, \( \text{H}_2 \) and \( \text{N}_2 \) are used as carrier gases, \( \text{NH}_3 \) and TMAl are reactants, and mixed into the reaction chamber from the inlet. The flow rates of \( \text{H}_2 \), \( \text{N}_2 \), \( \text{NH}_3 \) and TMAl are 50slm, 50slm, 20slm and 1slm, respectively. The temperature boundary condition of the wall is set to 2°C, the reactor pressure is 50Torr, and the susceptor rotation speed is 1000 rpm. Unless otherwise specified, these parameters remain unchanged during the simulation.
3. Results and Analysis

3.1. Influence of The Number of Heat Shields on Substrate Temperature

In order to study the influence of the heat shields on the heating efficiency and temperature, the number of heat shields is changed. The length of the heat shields is 148.7mm and the width is 2mm, and the interval between the heat shield is 2mm.

Figure 2. Substrate temperature distribution under different numbers of heat shields

Figure 3. Substrate temperature distributions of different lengths heat shields

Figure 2. shows the temperature distribution of the substrate under different numbers of heat shields. When the number of heat shields is increased from 0 to 4, the corresponding substrate temperature increases from 1227°C to 1380°C, and the standard deviation of temperature distribution is changed from 35.8°C rose to 54.4°C. It can be seen that the heat shields can effectively increase the surface temperature of the substrate, and the heating efficiency is proportional to the number of layers of the heat shields. It was found that when the number of layers of the heat shields exceeds 3, the increase of the substrate temperature slows down with the increase of the number of the heat shields. Taking the heating efficiency needed into account, it is reasonable to take three layers of heat shields.

3.2. Influence of the Length of Heat Shields on Substrate Temperature

Based on the above simulation results, the number of layers of the heat shields is 3, the length of the heat shields is 148.7mm, the width is 2mm, and the interval between the heat shields is 2mm. In order to investigate the effect of the length for the heat shields on the temperature, the length of the heat shields is reduced from the center of the substrate, that is, from left to right.

Figure 3. shows the temperature distributions of the substrate under different lengths of the heat shields. It can be seen that the longer the length of the insulation board, the higher the temperature of the substrate. As the lengths of the heat shields are changed from 230mm, 172mm, 114mm and 56mm to 28mm, the temperature STD in the substrate are 52.1, 40.2°C, 30.3°C, 21.4°C and 29.4°C. It is not difficult to find that the coefficient of substrate temperature STD is the best when the length of the heat shield is 56mm.

Figure 4. describes the distribution of flow field and temperature field in two different reactor, the convention reactor(a) and the optimized reactor. Figure 5. illustrates the distribution curves before and after substrate temperature optimization. The results show that the optimized flow field and temperature field are more suitable for the growth of AlN films. Through data comparison, the coefficient of substrate temperature STD was reduced by 45%, especially in the -200-200mm region, the coefficient of substrate temperature STD was reduced by 93%.
Figure 4. Distributions of flow field and temperature field in conventional reactor (a) and in optimized reactor (b)

Figure 5. Substrate temperature distributions in conventional reactor and in reactor with optimized heating structure

4. Conclusions
The effect of the number of layers and the length of the heat shields on the heating efficiency and temperature distributions in the substrate have been studied by establishing the model of a single-piece 18-inch MOCVD reactor. The results show that the number of layers of the heat shields is directly
proportional to the heating efficiency. And decreasing the length of the thermal shield can reduce the coefficient of substrate temperature STD. When the length of the heat shields is 56mm, the coefficient of substrate temperature STD is 21.41℃ and the STD is about 45% lower than the traditional susceptor. An area within substrate radius of 200mm, the coefficient of substrate temperature STD is 2.64℃ and the STD is about 93% lower than the traditional susceptor. The results obtained will provide theoretical basis for developing the heating structure of large-sized MOCVD reactor.

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