Numerical Study of Heating Structure in Cold-Wall MOCVD Reactor by Induction Heating

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Abstract. On the traditional heating structure of MOCVD reactor, the temperature distribution of substrate is nonuniform, which goes against the film growth. This paper focuses on the numerical calculation of the heating structure, by using SiC and graphite as the materials of the new susceptor and coupling with multifields. By adjusting the position and size of each of the ring body of graphite in the susceptor, the heat generation and heat transfer are changed, which leads to the approximately uniform heat conducted to the substrate, thus obtaining a more uniform temperature distribution. Compared to the traditional structure, under the same heating condition, the heating efficiency is improved about 9.1%, the uniformity of temperature distribution is improved more than 80%. This is very favorable for the growth of thin films.

1. Introduction

At present, the main technology for preparing nitride semiconductor materials is metal organic chemical gas phase (MOCVD). The rapid development of semiconductor technology in recent years has put forward higher requirements for the quality of semiconductor crystal thin films. Due to the complexity of the MOCVD technology, the film is restricted by many factors in the growth process. And the distribution of temperature uniformity in the substrate is particularly important, and it will directly affect the quality of the film [1,2,3,4,5]. At present, domestic and foreign scholars have done a lot of important work in this field.

Under the condition of induction heating, Xu et al. found the variation rule of changing the radial temperature on the surface of the graphite discs with changing the electric parameters of the coil in the simulation experiment [6,7,8]. Zhang et al. found that adjusting the concentric placement of
conventional graphite susceptor to eccentricity can effectively improve uniformity of the temperature distribution [9]. Li et al. designed a susceptor with grooved which change the direction of heat conduction in the susceptor [10].

By changing the single material composition of the traditional susceptor, the substrate heating structure with a diameter of 12 inches is investigated in this work, coupling with the electromagnetism, heat and fluid flow, and improving the temperature distribution of the substrate. The results obtained can provide theoretical and technical references for the development of large size MOCVD reactor.

2. Model of MOCVD reactor

Fig.1 showed that the model of MOCVD reactor. The reaction chamber is axisymmetric, which includes the wall, inlet, outlet, induction coils, substrates and alumina scaffolds. Fig.2 is a new susceptor structure given in this paper. As the whole model is axisymmetric, half of the structure of reactor is given in Fig.1 and Fig.2, respectively. The new susceptor consists of silicon carbide (SiC) and graphite.

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

In Fig.2, the areas denoted as A to G are ring bodies composed of graphite, which are embedded in SiC material. The susceptor height H is 25.4mm, the radius of the substrate R is 152.6mm. And the number of the coil is 17 in Fig.1. The electrical and thermophysical parameters of the model materials are all referred to the literature [11,12,13].

![Figure.2 New susceptor structure](image)

In the simulation, in order to improve the calculation speed and not affect the calculation results, we explain the following conditions:

1. regardless of the rotation of the susceptor;
2. don't care about chemical reactions between gases;
3. assume that the gas is in an ideal state;
4. the wall temperature is constant;

The gases in the reactor include, H₂, NH₃ and TMGa, which are mixed into the reaction chamber from the inlet. The flow rates of H₂, NH₃ and TMGa are respectively 40slm, 10slm and 10sccm, which remain unchanged in the simulation. In addition, the wall temperature boundary condition is set to 27℃. Because the growth of GaN film optimum temperature in 1050℃ or so, after repeated calculation, it is found that when the current frequency is 30.5kHz and current intensity is 200A, the substrate temperature can satisfy the growth temperature condition of GaN film.

3. Mathematical model of MOCVD reactor

The mathematical model is established by finite element method, and the heat conduction model is
coupled with the fluid model. For the convenience of solution, we simplify the electromagnetic equation:

$$\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial A}{\partial r} \right) + \frac{\partial^2 A}{\partial z^2} = j \mu \omega \sigma A - \mu J_{\text{col}}$$  \hspace{1cm} (1)$$

where $\omega$ is angular frequency of the alternating current, $\mu$ is magnetic permeability, $\sigma$ is the electrical conductivity, $J_{\text{col}}$ is the current density. $A$ is the magnetic vector potential.

Two-dimensional heat conduction equation:

$$\rho c_p \frac{\partial T}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) + \frac{\partial}{\partial z} \left( k \frac{\partial T}{\partial z} \right) + Q$$  \hspace{1cm} (2)$$

where $\rho$ is density, $c_p$ is specific heat, $t$ is time and $k$ is the thermal conductivity. $Q$ is the heat generated by electromagnetic induction:

$$Q = \frac{1}{2} \rho \frac{J_{\text{eddy}}^2}{\sigma}$$  \hspace{1cm} (3)$$

Where $J_{\text{eddy}}$ is the induced eddy current density and

$$J_{\text{eddy}} = -j \mu \omega \sigma A - J_{\text{col}} = -\frac{1}{\mu} \left( \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial A}{\partial r} \right) + \frac{\partial^2 A}{\partial z^2} \right)$$  \hspace{1cm} (4)$$

The fluid equations:

$$\frac{\partial \rho}{\partial t} + \text{div}(\rho U) = 0$$  \hspace{1cm} (5)$$

The fluid equation is coupled with the heat transfer equation:

$$\frac{\partial}{\partial t}(\rho \phi) + \text{div}(\rho U \phi) = \text{div}(\Gamma \phi \text{grad} \phi) + S_\phi$$  \hspace{1cm} (6)$$

Where div is gradient operator and div = $i \partial / \partial x + j \partial / \partial y + k \partial / \partial z$, $\rho$ density, $U = i u + j v + k w$, $\phi = u, v, w, T$, $\Gamma = \eta k / c_p$ or $\rho D_\phi$, ($k$ is thermal conductivity, $\eta$ viscosity, $c_p$ specific heat, $D_\phi$ binary diffusion coefficient) corresponding to momentum, species conservation or energy equations, respectively. $S_\phi$ is all other terms in each conservation equation, which is called source term.

Magnetic and thermal boundary conditions:

$$A = 0 \quad \text{at} \quad r = 0 \quad \text{and} \quad r^2 + z^2 = \infty$$  \hspace{1cm} (7)$$

Thermal boundary conditions between the wall and the substrate and the surface of the susceptor:

$$-k \frac{\partial T}{\partial n} = h(T - T_A) + \varepsilon \sigma_{\text{sb}} (T^4 - T_A^4)$$  \hspace{1cm} (8)$$

Where $n$ is the unit-normal to the surface, $\varepsilon$ is the effective emissivity, $\sigma_{\text{sb}}$ is the Stefan-Boltzman constant, $T_A$ is the temperatures of the walls of the reactor and the substrate. $h$ is the heat transfer coefficient.

The thermal boundary condition of axial symmetry:
\[
\frac{\partial T}{\partial r} = 0, \quad \text{at} \quad r = 0
\]  

(9)

Inlet: using the specified velocity boundary condition, the velocity value of the given inlet and the concentration value of the reaction gas.

Outlet: used the pressure boundary condition, the pressure is set as constant, and the other physical quantity is 0 in the export interface.

Wall: the wall temperature is given, and the velocity is set to non-slide boundary conditions.

And the initial temperature of the system is set to be 27°C.

4. Results and analysis

Fig.3 Temperature distributions of susceptor: conventional (a) and new (b)

Fig.4 shows that the Temperature distributions of two susceptor: the conventional susceptor (b) and the new susceptor (b). It can be seen that the traditional susceptor temperature distribution is very uneven. For the traditional susceptor, the whole susceptor is made of one material-graphite, so the thermal conductivity at each position is the same in the susceptor. While the new susceptor is made of graphite and SiC, every graphite-ring body is a heat produced body, and the heat generated by the graphite-ring body is transmitted through the area of SiC to the substrate. Because of the thermal conductivity of SiC is higher than that of the graphite, the susceptor of SiC materials area of heat transfer is faster.

By optimizing the size and position of the graphite ring body (the graphite ring body from left to right is named ring body A~G showed in Fig.2 which are rectangles in two dimension). In this simulation, the coordinates of the two points in the diagonal line of each rectangle are used to determine the positions of each body. It is found that when the coordinates of the bodies A-G are as follows: A((0, 0), (0.07*R, 0.55*H)), B ((0.13*R, 0), (0.2*R, 0.16*H)), C((0.36*R, 0), (0.39*R, 0.12*H)), D((0.51*R, 0), (0.54*R, 0.08*H)), E((0.75*R, 0), (0.78*R, 0.16*H)), F((0.84*R, 0), (0.87*R, 0.12*H)), and G((0.93*R, 0), (R, 0.67*H)), substrate temperature uniformity is the best.

Fig.4 Temperature distributions of substrate: conventional and optimized

Fig.5 shows the temperature distributions of substrate on the conventional susceptor and the optimized susceptor. Compared with the conventional structure, the new susceptor has better temperature uniformity. The heating efficiency of the new structure is significantly higher than that of the conventional structure. Under the same heating conditions, the average substrate temperature and
standard deviation of the new susceptor and the traditional susceptor are: new structure: 1041 °C, 6.7 °C; conventional structure: 954 °C, 34 °C.

5. Conclusion
In this paper, designed a new heating structure in the MOCVD reactor. Compared with the conventional heating structure, the susceptor in the new structure is made of two materials which are graphite and SiC, while only one material-graphite is used in the conventional heating structure. By optimizing the new heating structure, the uniformity of the temperature distribution is improved more than 80%.

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