Numerical Investigation of Pallet Structure with Annular Slot in MOVPE Chamber

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Abstract. A pallet structure with an annular slot is proposed in the perpendicular MOVPE chamber by electromagnetic heating. Compared with the conventional pallet, the shape of the slot changes the directions of the thermal conduction in the pallet, which makes the temperature distribution of the substrate more uniform. The optimized pallet structure which makes the most uniform temperature profile of the substrate is also given. In addition, the intervals of the applied parameters such as the current frequency, current strength and coil turns which keep the stable change of the substrate temperature are also obtained, by analyzing the change of the substrate temperature with the parameters. When one of the parameters is changed in the interval, the temperature magnitude can be adjusted while ensuring a certain uniformity of the temperature. This is beneficial to control the growth of the thin film.

1. Introduction

Gallium nitride (GaN) is a wide-gap semiconductor and has been widely used in blue-green opto-electronic devices [1]. Presently, MOVPE has been the commonly used method in growing high-quality films and large-scale production compatibility [2], in which electromagnetic heating is always used to produce the temperature needed for reactions in the MOVPE chamber. So far, the electromagnetic heating which is used in crystal growth has been widely studied. Chen showed that by maintaining current strength in the coils, the highest temperature was improved with increased the electric current[3]. Li et al. analyzed the influences of the relative position between the coils and the middle section of the pallet, the the coil radius, and the height of the pallet on heating in the perpendicular MOVPE chamber [4]. However, there have been few studies on the influence of the shape of the pallet on the temperature profile in the chamber. The main objective of the present study is to give a pallet structure with an annular slot and optimize the structure which makes the substrate temperature uniform. Furthermore, the intervals of the parameters such as the current frequency, current strength and coils which make the substrate temperature stably change are determined.

2. Mathematical model

A numerical method has been used which consists of calculation of the frequency time-harmonic magnetic field by electromagnetic heating and calculation of the heat-field distribution. In the work, the magnetic potential vector theory is used for calculating the temperature profile of the electromagnetic heating with an axisymmetrical conduction-radiation model. The Maxwell equations and boundary
conditions used are referred to Ref. [3]. The temperature profile in the chamber can be obtained by using a heat equation:

$$c \rho \frac{\partial T}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( k_r r \frac{\partial T}{\partial r} \right) + \frac{\partial}{\partial z} \left( k_z \frac{\partial T}{\partial z} \right) + q_H \tag{1}$$

where $c$ is the heat capacity, $\rho$ is the density, $k_j$ is the thermal conductance of the material $j$, $t$ is time and $q_H$ is the eddy-current-generated thermal power density caused by the induction which can be obtained from:

$$q = \frac{1}{2} \sigma \omega^2 A_0 A_0^* \tag{2}$$

Where $A_0^*$ and $A_0$ are conjugate, $A_0$ is the magnetic vector potential, $\omega$ and $\sigma$ are the angular frequency, electrical conductivity, respectively. The symmetric condition is:

$$\frac{\partial T}{\partial r} = 0, \quad \text{as} \quad r = 0 \tag{3}$$

As the flow rate of the gases has little effect on the substrate temperature [5], and the influence of free convection on the temperature changes in the substrate is small [6], the flow rate of the gases and free convection are ignored. Thus, a coupling radiation-conduction boundary condition is applied on the external surfaces of the pallet:

$$- k_m \frac{\partial T}{\partial n} = - k_j \frac{\partial T}{\partial n} + q_{rad}, \quad m \neq j \tag{4}$$

Where $k_m$, $k_j$ are the heat conductivity of the pallet and of the gas, respectively, $\vec{n}$ is the unit normal outward vector to the surface of the pallet and $q_{rad}$ is the heat radiation from the pallet to surrounding walls.

The heat conduction in the chamber wall is described by the equation:

$$c_w \rho_w \frac{\partial T}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( k_r r \frac{\partial T}{\partial r} \right) + \frac{\partial}{\partial z} \left( k_z \frac{\partial T}{\partial z} \right) \tag{5}$$

Where $c_w$, $\rho_w$ and $k_w$ are specific heat, density and thermal conductivity of chamber wall, respectively. The relevant boundary condition of equation (5) is referred to [7]. And the starting temperature of the model is set to be 27°C.

![Figure 1. Model of pallet in chamber](image)

The electromagnetic field is analyzed by a two-dimensional model including these: the graphite pallet, the sapphire substrate which is on the pallet, the wall surfaces of the chamber, the coils, the upper flange, the down flange which are displayed in Fig.1. A FEM(finite element method: ANSYS software) has been used. Detailed mesh generations are referred to Ref.[4]. The current in the coil is assumed to be time-harmonic, and the distribution of the current in the coil is uniform.

During film growth, hydrogen ($H_2$) is usually used as the carrier gas and the objective of the paper lies in the study of temperature profile of the substrate, other organometallic compounds are ignored in
the flow. And the gas is assumed transparent to the infrared emission because of its relatively short path in MOVPE chambers. The physical parameters of H$_2$ such as the thermal conductivity, thermal capacity are seriously dependent on the temperature [7]. As the rate of the gas flow is unchanged, the density of H$_2$ is set to be 0.0819kg/m$^3$. In this model, the influences of the changing temperature on the materials of each part in the chamber are also considered [8].

3. Analysis of Results
Two kinds of pallet structures are shown in Figure 2, where (a) is the one without slot and (b) is the one with an annular slot. In the perpendicular MOVPE reaction chamber, a column-shaped pallet made of graphite is usually used, and the substrate is placed on the upper surface of the pallet, which is shown in Figure 2 (a). The coils are distributed around the outside chamber wall. Because of the skin-effect, the majority of the induced current is distributed in the skin depth of the pallet. Thus the majority of the heat generated in the pallet is also inside of the pallet, and the temperature inside the pallet is higher than that near the pallet center area. So the temperature profile of the substrate is extremely non-uniform. In order to solve this issue, the pallet with an annular slot shown in Figure 2 (b) is put forward. The induction-generated heat in the pallet is divided into two parts by isolation of the slot, one of which is inside the pallet above the slot and the other is under the annular slot. The former heats more uniformly distributed near the edge of the substrate above the slot. The latter isolated by the slot, can change the heat transfer directions along the bottleneck to the region near the center of the substrate. And therefore, the central region of the substrate gets more heat, and the region near the side of the substrate gets less. Consequently, a more uniform temperature profile of the substrate can be achieved, which will be illustrated in the work below. For the sake of discussion, several parameters shown in Figure 2 are defined as:

$h$: the pallet height and $h$=50.8mm, $H$: the distance between the upper surface of the annular slot and the upper surface of the pallet, $L$: the slot depth, $W$: the slot height.

![Figure 2. Schematic of two kinds of pallet structures: (a) pallet without slot and (b) pallet with annular slot](image)

3.1. Optimized slot in pallet
The optimal location and size of the slot in the pallet which makes the substrate temperature the most uniform can be obtained, by comparing the temperature profiles in the substrate on the pallet with the slot of various locations and sizes (mainly by changing $L$, $H$ and $W$) under the conditions that current frequency $f$=30KHz, current strength $I$=300A and coil turns $n$=6. Figure 3 shows the temperature profile in the pallet without slot (a) and with the optimized slot (b). It can be seen that the temperature in the optimized pallet is higher than that in the pallet without slot. Meanwhile, the temperature in the substrate on the pallet without slot is higher in both sides of the substrate than that in the center, while the temperature contours in the substrate on the optimized pallet is almost smooth. This is due to the slot which divides the generated heat in the pallet into two parts: the one part accumulates on the upside and the other downside of the slot. They are transferred by conduction to the edge and center area of the substrate and heat them, respectively. In other words, the directions of thermal transfer are changed by the slot, and the slot makes the heat in the pallet redistribute so that the uniformity of the temperature in the substrate is highly improved.
3. Temperature profile in substrate and pallets

(a) pallet without slot; (b) pallet with optimized slot: L=0.6r, H=0.15h, W=0.08h

Figure 4 shows the temperature profile of the substrate on pallets with optimized and without slot. It can be obtained that compared with the pallet without the slot, under the same conditions, the average temperature is raised from 915°C to 941°C, the temperature profile range decreases from 36.9°C to 5.72°C, and the standard deviation of temperature profile decreases from 9.94°C to 0.8°C. The fluctuation of the temperature is less than 1°C (not including the edge of the substrate).

However, when the applied parameters such as the current frequency, the current strength and the coil turns change, the temperature profile in the optimized pallet will change accordingly, and the uniformity of the temperature of substrate can be destroyed. In the following, the stability of the temperature changing with the three parameters is studied. Thus, we define the stability as: if one of the three parameters changes in a certain range, the standard deviation of the temperature of the substrate is less than 2.5°C, then the effect of the parameter on the uniformity of the temperature is stable, and the range is called the stable interval.

3.2. Analysis of stability of applied parameters

3.2.1. Effect of current frequency f on stability

For the convenience of analysis, in the following study, the following parameters are selected as the base condition: the current strength I=300A, current frequency f=30KHz, and the turns of coil n=6. When one of the three is changed, the other two are kept constant.

The temperature profile in the pallet and the substrate under four frequencies are shown in Figure 5, and the temperature profile in the substrate under eight frequencies (a) and their numerical characteristics (b) are indicated in Figure 6. It is observed that the temperature is proportional to the current frequency. But the uniformity of the temperature profile is destroyed with the frequency increasing or decreasing. This is because that the skin depth increases with the decreasing frequency (such as f=10KHz or 20KHz), and the relatively high temperature region in the pallet increases. The heat from the region under the slot to the center of the substrate increases correspondently. So the temperature of the substrate is higher in the center and lower in both sides shown in Figure 5 (a) and (b). On the contrary, when the frequency increases, the skin depth decreases accordingly, and the higher temperature region in the pallet decreases and moves towards both sides of the pallet. The temperature in the region of the pallet on the upside of the slot increases with the increasing frequency, while the heat from region under the slot to the center of the substrate gets lower relatively, which results in the lower temperature in the center and higher in both sides of the substrate. Moreover, the average temperature increases with the increasing frequency, but the incremental rate decreases. It can be found
that when the frequency changes in the interval [25KHz, 35KHz], the influence of the frequency on the temperature is stable.

Figure 5. Temperature profile in pallet and substrate under various frequencies(KHz)

3.2.2. Effect of coil turns n on stability

Figure 7 shows the temperature profiles of the substrate under various turns of coil (a) and their number characteristics (b). It can be seen that the average temperature rises gradually with the increasing of coil turns, however its increase rate decreases. In addition, the temperature standard deviation increases with the decrease of the coil turns (such as n=4 or 5) or increase (such as n=7, 8 or 9). When coil turns n= 5, 6, or 7, the effect of the coil on the uniformity of the temperature is stable, shown in Figure 7(b).

3.2.3. Influence of current strength I on stability

As the current strength changes, it can be found from Figure 8 that the temperature of the substrate increases linearly with the increased current strength, furthermore the average temperature increases by about 36°C as the current strength increases by 20A. However, the standard deviation of the substrate temperature grows with increasing I (I > 300A) or decreasing (I < 300A). It is observed that the effect of I on the temperature is stable under the condition that I changes in the interval [240A, 340A].

Figure 8. (a)Temperature profiles of substrate under various I. (b)their number characteristics
4. Conclusion
A pallet structure with an annular slot is put forward. With the basic parameters unchanged, uniform temperature profile of the substrate is achieved by changing the size and the location of the slot in the pallet. In addition, it is found that the temperature of the substrate on the optimized pallet is directly proportional to the current strength, current frequency, and the coil turns. Furthermore, the effects of these basic parameters on the uniformity of the substrate have a certain stability. That is to say, if we change one of the three basic parameters and keep the other two constant, the interval which the current frequency makes the temperature of the substrate stable is [25KHz, 35KHz], the interval which the current strength does is [240A, 340A], and the turns of the coil which makes the substrate temperature stable is 5~7 turns. The simulated results prove that one basic parameter can be changed to adjust the substrate temperature for the benefit of controlling the growth of the thin film.

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