NUMERICAL SIMULATION AND ANALYSIS OF PROCESS PARAMETERS OF GAN-MOCVD REACTOR

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ABSTRACT

In this work, the GaN-MOCVD reactor with vertical spray structure is simulated, and a numerical solution to the steady flow in low pressure with substrate axisymmetrical rotating is obtained by the computational fluid dynamics software. The temperature field, flow field, operating pressure, rotation speed of substrate are analyzed, and process conditions are optimized which can make the flow field in reactor more stable to ensure the thickness uniformity of deposited thin film. This paper not only provides an effective solution for high-quality epitaxial growth, but also provides a theoretical basis for the follow-up experiment and equipment improvement.

1.INTRODUCTION

III-V compound semiconductor thin film based on Gallium nitride is important third generation semiconductor material, which is widely used in the manufacture of blue-violet light emitting diodes, semiconductor lasers and high-frequency electronic equipments [1-2] with high power. Metal organic chemical vapor deposition (MOCVD) technology is a cost-effective way [3-4] to produce the film with advantages of large epitaxial area, good reproducibility, accurate component control and high deposition rate. In the process of chemical vapor deposition, the gas flow, heat distribution and concentration distribution above the substrate are vital to the growth rate and thickness uniformity of thin film [5-9]. In order to obtain uniform composition and film thickness, the gas flow must be laminar, vortex near the substrate does not occur, gas flow in the direction parallel to the substrate has uniform temperature field and in vertical direction with a high temperature gradient, and the particles concentration near the substrate should be as uniform as possible. Generally coefficient variation less than 5% is considered to be qualified in practical projects.

CFD (Computational Fluid Dynamics) is an indispensable tool for the development of MOCVD equipment. Three-dimensional simulation of flow field in MOCVD reactor has been paid growing attention [10-12], and many manufacturers have made great benefits in researching reactor structure, shorting design cycles, reducing development costs [13-15], etc.

This paper investigates the MOCVD design by CFD technology, characteristics of fluid dynamics with the gas inlet flow rate, operating pressure, and rotation speed of substrate change within a certain range are studied, it also draws corresponding distribution rules in the flow field, temperature field and thin film deposition rate in the reactor. According to the simulation results and application of fluid mechanics and thermodynamics [16], transport processes and external operation parameters are analyzed and discussed, Some valuable new results are obtained by calculating, and improvements for the flow stability in MOCVD reactor are proposed.

2.NOMENCLATURE

μ	[Pa·s]	Viscosity
$\vec{v}$	[m/s]	Components of the velocity vector
ρ	[kg/m^3]	Density
t	[s]	Time
P	[Pa]	Pressure
u	[m/s]	Components of the velocity vector in the x direction
v	[m/s]	Components of the velocity vector in the x direction
w	[m/s]	Components of the velocity vector in the z direction
S_u	[pa/m]	Pressure source term in the x direction
S_v	[pa/m]	Pressure source term in the y direction
S_w	[pa/m]	Pressure source term in the z direction
x	[m]	Cartesian axis direction
y	[m]	Cartesian axis direction
z	[m]	Cartesian axis direction
T	[K]	Temperature
K	[W/(m·K)]	Thermal conductivity
C_p	[J/(Kg·K)]	Specific heat at constant pressure
S_T	[J/(m^3·s)]	Heat source term

3.THEORETICAL FOUNDATION

The fluid flow is defined by the laws of conservation of mass, momentum and energy. These laws are expressed in terms of partial differential equations which are discretized with a finite element based technique.

1. Continuity Equation

From the law of conservation of mass law comes the continuity equation:

$$\frac{\partial \rho}{\partial t} + div(\rho \vec{u}) = 0 \tag{1}$$

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where ρ, t and $\vec{u}$ are the density,time and the velocity vector.

2. Momentum Equation

$$\frac{\partial(\rho u)}{\partial t}+div(\rho u\vec{u})=div(\mu\ grad\ u)-\frac{\partial p}{\partial x}+S_u \quad (2)$$

$$\frac{\partial(\rho v)}{\partial t}+div(\rho v\vec{u})=div(\mu\ grad\ v)-\frac{\partial p}{\partial y}+S_v \quad (3)$$

$$\frac{\partial(\rho w)}{\partial t}+div(\rho w\vec{u})=div(\mu\ grad\ w)-\frac{\partial p}{\partial z}+S_w \quad (4)$$

Where $grad() = \partial()/\partial x+\partial()/\partial y+\partial()/\partial z$,the symbols of S_u, S_v, S_w are generalized source terms of momentum equation, $S_u = F_x + s_x$, $S_v = F_y + s_y$, $S_w = F_z + s_z$,and s_x, s_y, s_z are small amount expressed by

$$s_x=\frac{\partial}{\partial x}(\mu\frac{\partial u}{\partial x})+\frac{\partial}{\partial y}(\mu\frac{\partial v}{\partial x})+\frac{\partial}{\partial z}(\mu\frac{\partial w}{\partial x})+\frac{\partial}{\partial x}(\lambda\ div\,\vec{u}) \quad (5)$$

$$s_y=\frac{\partial}{\partial x}(\mu\frac{\partial u}{\partial y})+\frac{\partial}{\partial y}(\mu\frac{\partial v}{\partial y})+\frac{\partial}{\partial z}(\mu\frac{\partial w}{\partial y})+\frac{\partial}{\partial y}(\lambda\ div\,\vec{u}) \quad (6)$$

$$s_z=\frac{\partial}{\partial x}(\mu\frac{\partial u}{\partial z})+\frac{\partial}{\partial y}(\mu\frac{\partial v}{\partial z})+\frac{\partial}{\partial z}(\mu\frac{\partial w}{\partial z})+\frac{\partial}{\partial z}(\lambda\ div\,\vec{u}) \quad (7)$$

For incompressible fluid that viscosity is constant, $s_x = s_y = s_z = 0$.

3. Energy Equation

$$\frac{\partial(\rho T)}{\partial t}+div(\rho\vec{v}T)=div(\frac{K}{C_p}gradT)+\frac{S_T}{C_p} \quad (8)$$

where C_p, T, K are specific heat at constant pressure,temperature and thermal conductivity. S_T is the heat source.

4. State Equation

The detail form of the state equation is determined by specific situation:

$$\rho = f(p,T) \quad (9)$$

4. MATHEMATICAL MODEL AND VERIFICATION

4.1 FLUID DYNAMICS CHARACTERISTICS AND MESH MODEL OF MOCVD REACTOR

Carrier gases are generally N2 and H2. III group Ga source uniformly sprayed into reactor through vertical pipes, V group N source flow into the reactor from tapered fumaroles and central observation window, and change direction by a baffle. The reactor model and gas flow diagram are shown in Figure 1. After mixed gas flowing through heated substrate, chemically react to produce monomer molecules, these monomer molecules will collide, condense, crystallize and grow into a molecular cloud of particles, heterostructure thin film eventually forms on the substrate surface. The molecular cloud which is not deposited on substrate will leave the reactor with reactants, by-products and carrier gas through the exhaust flow channel on sidewall.

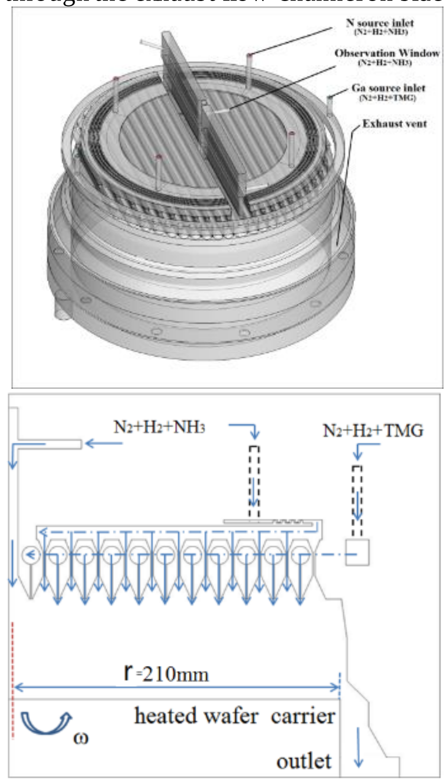


Figure 1 Reactor model and gas flow diagram of GaN-MOCVD

As shown in Figure 2, hexahedral mesh is used and local refinement is used in where flow rate and temperature gradient is large. To ensure numerical accuracy of flow field in the reactor, mesh density is basically same in intersection. Total number of grids are 10294813.

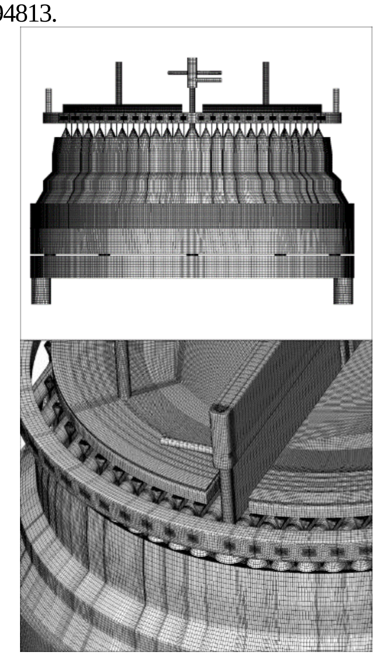


Figure 2 Reactor mesh and local grid diagram of GaN-MOCVD

4.2 DESCRIPTION OF DESIGN SCHEMES AND NUMERICAL SIMULATION PARAMETERS

To simplify the complex simulation process and make the calculation more efficient, we make the following assumptions on the premise that the main results are not affected.

(1) In view of the growth of semiconductor material with a continuous steady-state process under the control of mass transmission. Experimental schemes are shown in Tab.1, boundary conditions are set on the basis that flow rate of carrier gas, operating pressure, temperature and rotation speed of the substrate are changed in a certain range.

Tab.1 Experimental Scheme

Susceptor Temperature（K）	1273.15	Susceptor rotational speed（rpm）	1200	Static pressure（torr）	200
Total gas flow (slm)	1260	Molar percentage of H_2（%）	4.6	Molar percentage of TMG（%）	0.22
Molar percentage of NH_3（%）	21	Molar percentage of N_2（%）	74.18		

(1) Laminar flow is adopted due to the Reynolds number is less than 2300.

(2) The graphite plate is with good thermal conductivity, the temperature difference within the susceptor is very small, considering the temperature is constant.

(3) Inner and outside walls are along with water cooling system that make temperature set to 323.15K. And non-slip boundary condition is applied.

(4) Adopt pressure-outlet boundary condition that a given outlet static pressure is 0 Pa.

(5) As shown in **Figure 3**, there are 38 wafers which size is 2 inches circumferentially arranged on the substrate, and the distance from the center of the substrate is: a=0.005m, b=0.205m.

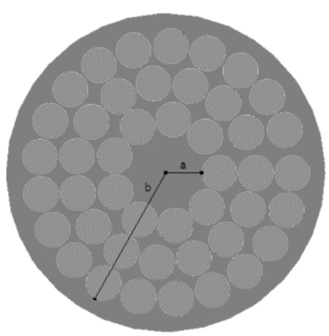


Figure 3 Susceptor model in MOCVD reactor

5.ANALYSIS AND DISCUSSION

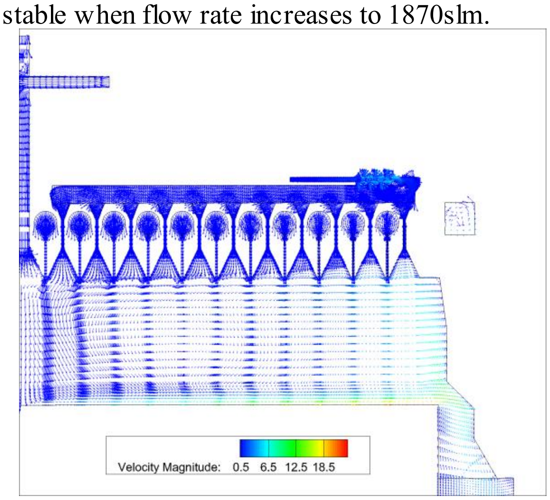
The important parameters to evaluate the quality of epitaxial growth technology are: crystal growth rate; uniform components; doping concentration and thickness; steep heterogeneous interface; utilization rate of various kinds of source materials. So we need to clearly understand the flow states of the reactants in reactor. And in order to form uniform temperature field and flow field in the vicinity of substrate, which requires a good control of transmission state of the reactants. In the process of MOCVD, there is thermal diffusion caused by temperature gradient which namely thermal buoyancy phenomenon. On the one hand, it can make the by-product particles away from growth zone to improve the quality of thin film, on the other hand, it also makes the growth areas difficult to be reached, so film growth rate decreases.In order to study this phenomenon, this paper focuses on the effects of process parameters on the flow field, temperature field, and deposition rate.

5.1 IMPACTS OF GAS FLOW INLET RATE ON THE DISTRIBUTION OF HEAT FLOW FIELD AND DEPOSITION RATE

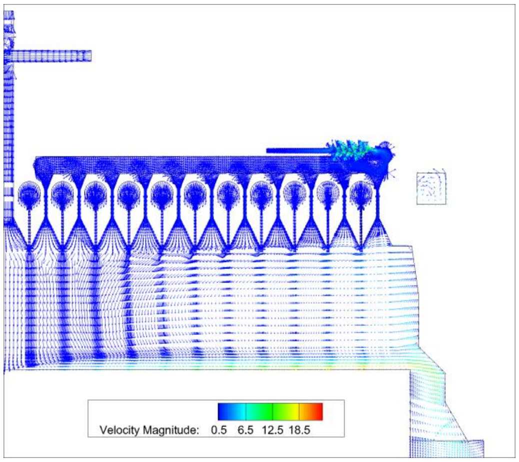
Gas flow inlet rate is a very important process parameter, it not only determines the rate of epitaxial growth, but also has an important influence on the flow field and temperature field in the reactor. In this experiment, Conditions for the simulation are changing the gas flow inlet rate: 303slm, 632slm, 1260slm, 1870slm, 2170slm, and 2450slm.

As shown in Figure 4, when flow rate is 303slm and 632slm, vortex appears in the flow field above graphite plate, which is induced by thermal buoyancy and rotation. When flow rate is small, the paraxial gases are extrapolated in the joint effect of viscous force and radial pump, so that a large toroidal vortex formed near the base. Vortex also appeared at the bottom of base, which is caused by the change of flow channel.

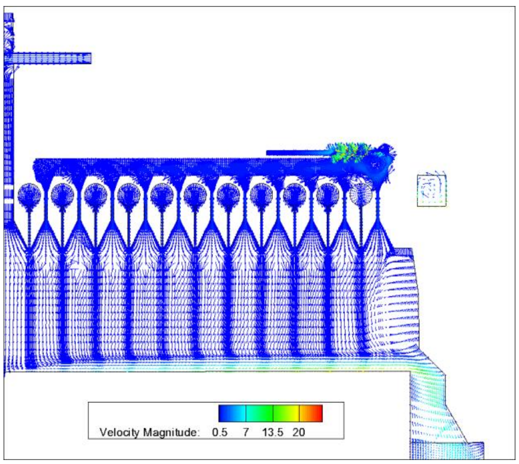
The vortex above the base of graphite plate make the reaction product remain in reactor ,and it is not conducive to the crystallization quality of thin film. With flow rate increasing, the vortex is compressed to the top left of graphite plate susceptor, now it belongs to the plug flows, which are caused by the specific design of this reactor sprayer. We can conclude that the increase of flow rate is beneficial to the stability of flow field in the reactor, and the flow field has been stable when flow rate increases to 1870slm.



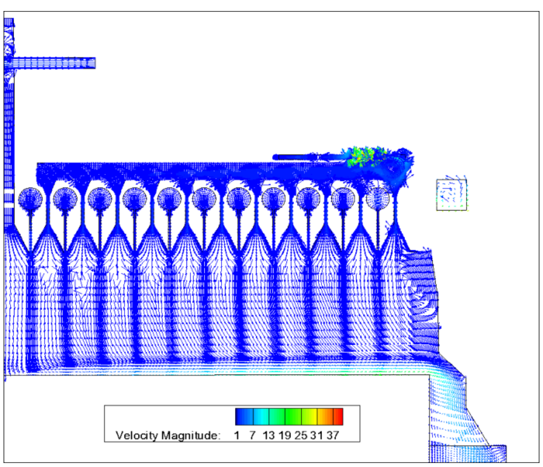
(a) 303 slm



(b) 632 slm



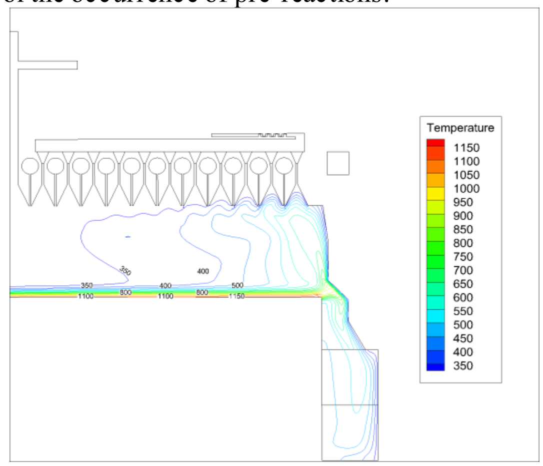
(c) 1260 slm



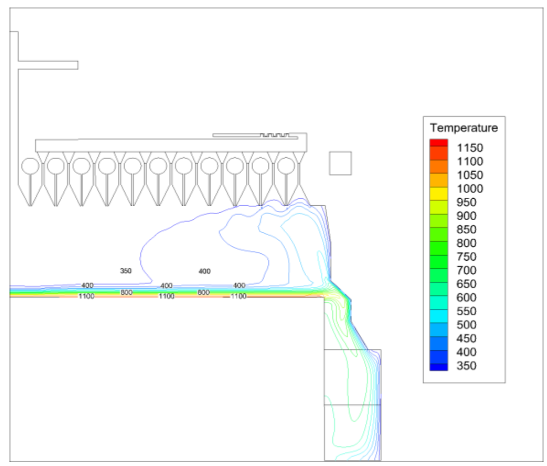
(d) 1870 slm

Figure 4 The vector diagrams under different flow rates

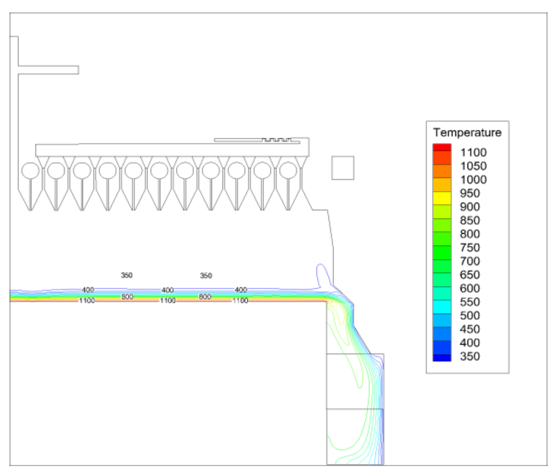
As shown in **Figure 5**, at the cases of flow rate of 303slm and 632slm, there exists a great temperature gradient in reactor, and the temperature on the top of susceptor is high due to the influence of rotation induced vortex. In the process of film growth, pre-reactions would occur in high-temperature region and affecting the crystalline quality. With the flow inlet rate increase, high-temperature region continues to decrease until only a thin layer which substantially parallels to the substrate exists on the surface, indicating that with the increase of flow rate, the thermal buoyancy effect has been effectively suppressed, which is conducive to the growth of thin film. Temperature change is more obvious in the case of high flow rate and it is beneficial to control the occurrence of pre-reactions.



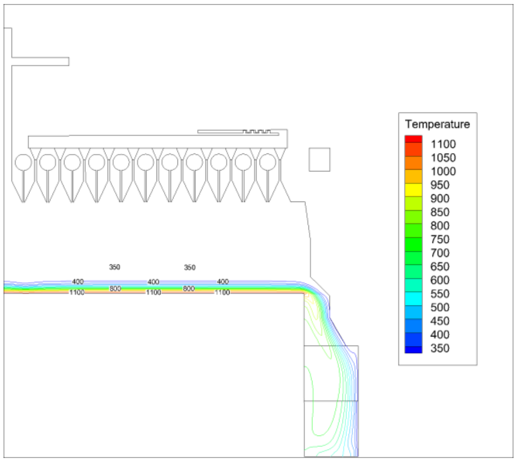
(a) 303 slm



(b) 632 slm



(c) 1260 slm



(d) 1870 slm

Figure 5 The temperature contours under different flow rates

Figure 6 shows the distribution trend and film deposition rate with the increase of flow rate. When gas flow rate is low, there is no enough source gas can enter so that deposition rate is relatively low. It appears mutation when gas flow rate is 303slm and 632slm, because internal maelstrom caused the deposition component is low, so that the deposition rate decreases. Upturned edge of 1260slm to 2450slm is caused by the flow channel crunch, but in the growth transition area is relatively flat.

We can conclude that the deposition rate increases linearly with the increase of flow rate, but it is not a multiple of increase. But when gas flow rate is too high, the majority of the reactant will discharged from the pump, the consumption of source material increases.

As it can be seen in **Figure 7**, the uniformity of deposition rate is gradually increased, and the variation coefficient of 632slm has been reduced to less than 5%, but when the flow rate is too high to reach 2450slm, it has a certain effect on the uniformity of deposition rate.

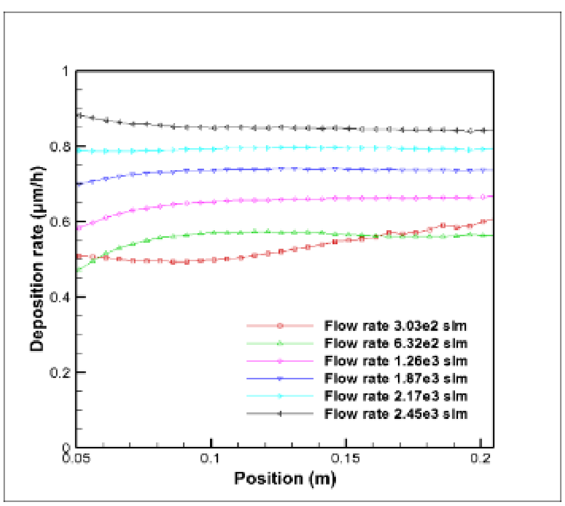


Figure 6 Deposition rate distribution on the substrate surface under different flow rate

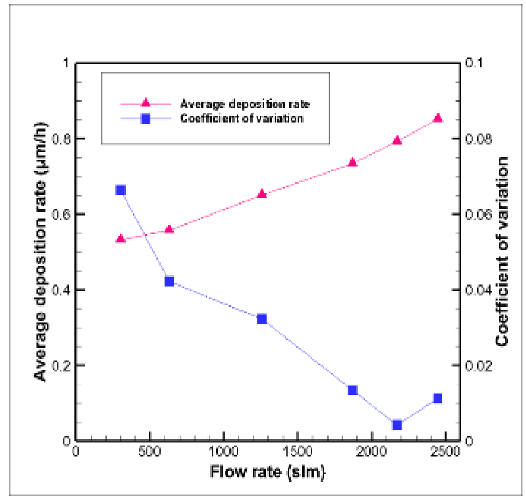
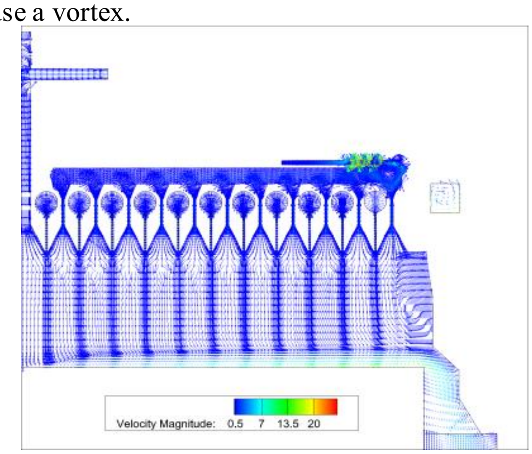


Figure 7 Average deposition rate and coefficient of variation under different flow rate

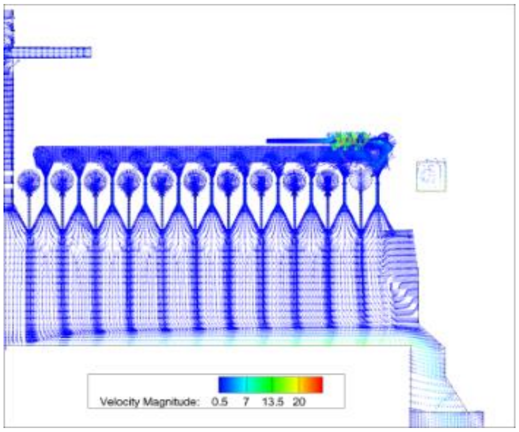
5.2 IMPACTS OF THE ROTATION SPEED OF SUBSTRATE ON THE DISTRIBUTION OF HEAT FLOW FIELD AND DEPOSITION RATE.

The ultimate goal of research of transport process is to obtain a uniform temperature field and concentration field in the vicinity of substrate. In order to improve the quality of products, most advanced MOCVD devices are used to improve the uniformity of deposited films by using rotating substrate. Conditions for the simulation are changing the rotation speed of substrate: 600rpm, 800rpm, 1000rpm, 1200rpm, 1400rpm and 1600rpm.

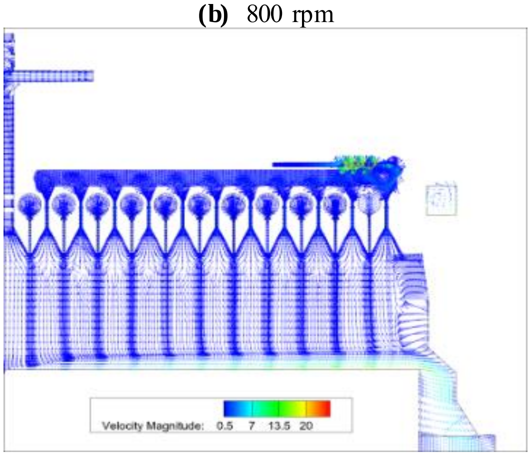
Figure 8 clearly shows the impacts of rotation speed of substrate on the gas flow. When at low rotation speed of 600rpm to 800rpm, rotating vortex is small and belonging to the plug flow, the turntable plays the role of pulling down airflow. with the rotation speed increase, reverse pressure gradient caused by the action of radial pump lead to the gas flow turn into a vortex flow, and that form an annular vortex around the wall near substrate. With the rotation speed increases, the vortex gradually turn into a large annular vortex, so that the high rotation speed of the substrate is more likely to cause a vortex.



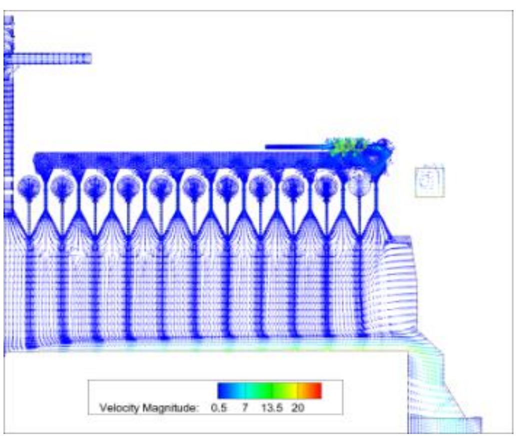
(a) 600 rpm



(b) 800 rpm



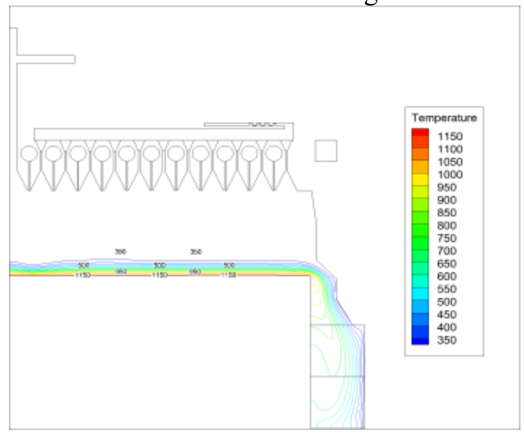
(c) 1000 rpm



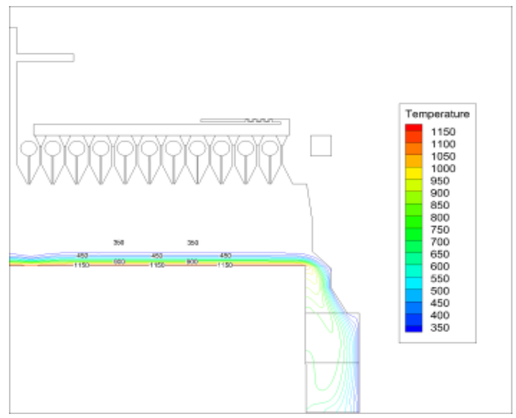
(d) 1200 rpm

Figure 8 The vector diagrams under different rotation speeds

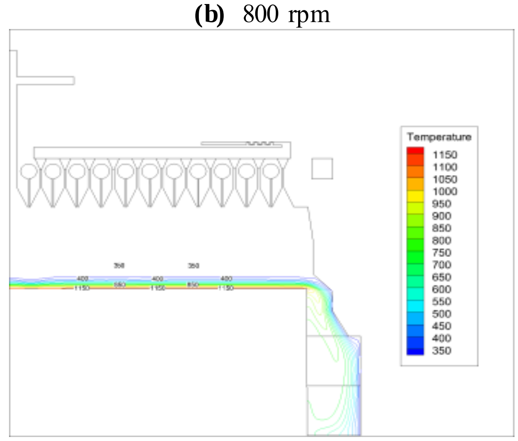
Figure 9 shows when other conditions remain unchanged, the rotation changes the state of gas flow, but it did not play a destructive effect on temperature layer on the substrate surface. And the distribution of high-temperature region which substantially parallel to the surface of susceptor is uniform, which is conducive to the film growth. The temperature difference near the surface increases with the rotation speed increase, but the high temperature layer thickness decreases which may be due to the axial pumping action caused by the rotation of the susceptor, and the temperature distribution on base surface gets more stable.



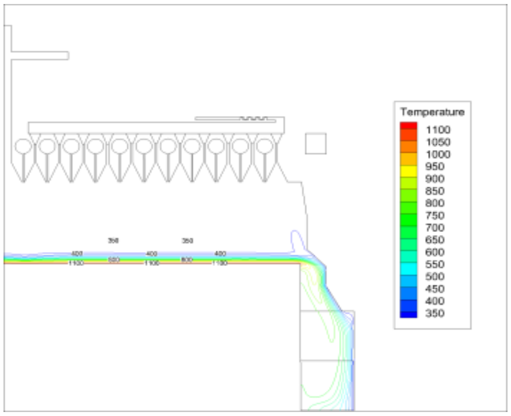
(a) 600 rpm



(b) 800 rpm



(c) 1000 rpm



(d) 1200 rpm

Figure 9 The temperature contours under different rotation speeds

Figure 10 presents the substrate deposition rate distribution trend and film deposition rate with the rotation speed increases. With the increase of rotation speed, the deposition rate increases, but increasing rate gradually decreases, which is consistent with the literatures [17-18]. It also shows in **Figure 11** that the uniformity of deposition rate gradually increase, and the rate of increase is gentle. When rotation speed is 1000rpm, the coefficient of variation has been less than 5%.

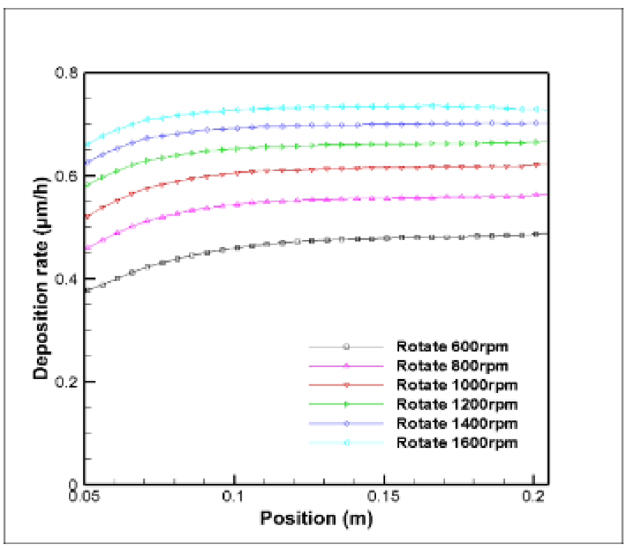


Figure 10 Deposition rate distribution on the substrate surface under different rotation speeds

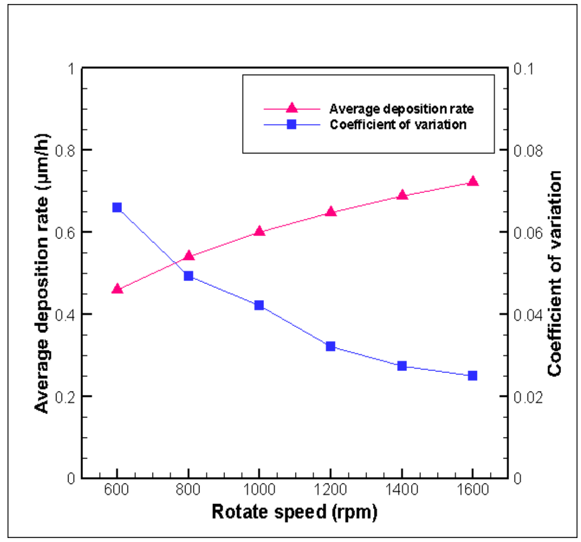


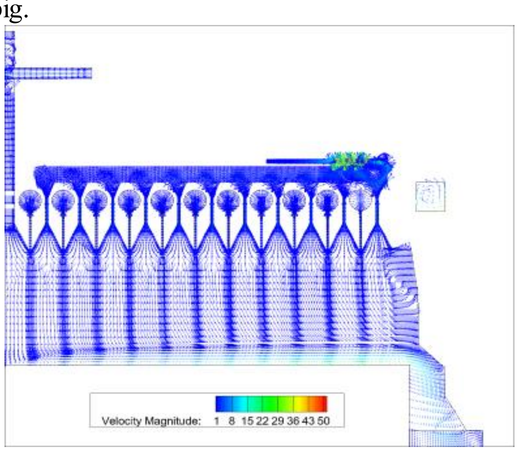
Figure 11 Average deposition rate and coefficient of variation under different rotation speeds

5.3 IMPACTS OF OPERATING PRESSURE ON THE DISTRIBUTION OF HEAT FIELD AND DEPOSITION RATE

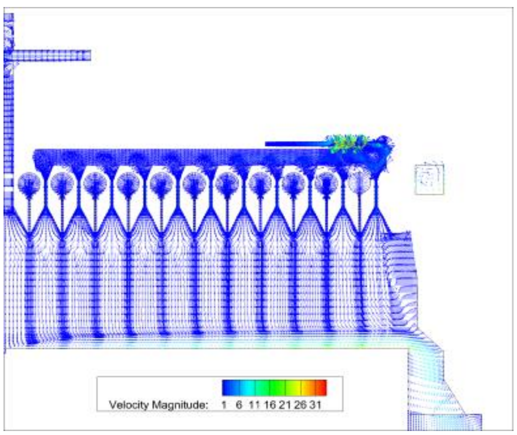
It is an important technique to improve the uniformity of thin film by controlling operating pressure in reactor. In the process of atmospheric MOCVD [19], component concentration has drastic changes along with the gas flow direction due to the continuous depletion of reactants, which is very easy to cause the uneven of growth layer thickness. Conditions for the simulation are changing the operating pressure: 100torr, 150torr, 200torr, 300torr, 400torr and 500torr.

Figure 12 shows when pressure is 100torr and 150torr, flow field above the susceptor is stable, which belongs to the piston flow; When pressure increases to 200torr, vortex expanded above the left side of graphite base; When pressure increases to 300torr, the vortex move to the right and become large, and the flow field has become less stable. This phenomenon can be explained by the dimensionless number Gr/Re^2, which is the relative size of thermal convection and forced convection. As the other conditions are the same, from the ideal gas equation of state, $\rho = PM_W/RT$, that density ρ is proportional to the pressure P, when the pressure is reduced, the density decreases. Since the inlet flow rate Q remains unchanged, ρv remained unchanged, if ρ reduced, the inlet flow v increases. In the case of low pressure, the viscosity μ is basically unchanged, Re can be thought remains unchanged. The definition of Gr number shows that $Gr \propto \rho^2$, and by the ideal gas equation of state $\rho \propto P$, $Gr \propto P^2$ can be obtained. So when the pressure is reduced, the Gr drops, the Gr/Re^2 also drops, so the influence of the thermal convection become weak, and the vortex caused by the thermal convection will also disappear. In contrast, when the pressure increased, the Gr/Re^2 rises, the influence of the thermal convection enhanced, and the vortex gets more obvious.

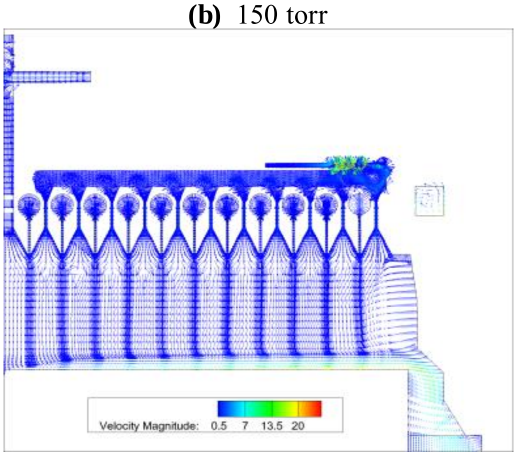
Figure 12 further proves the effect of pressure on the temperature field in reactor. It is showed that low pressure is conducive to the stability of flow field, and it is good for the uniformity of film growth. But pressure is not the lower the better, in the case of pressure is too low, the gas flow rate will be very big.



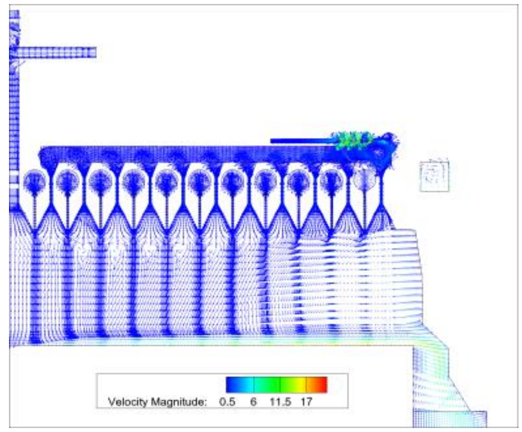
(a) 100 torr



(b) 150 torr



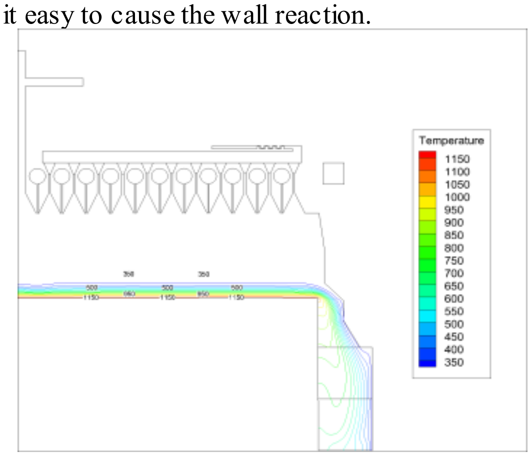
(c) 200 torr



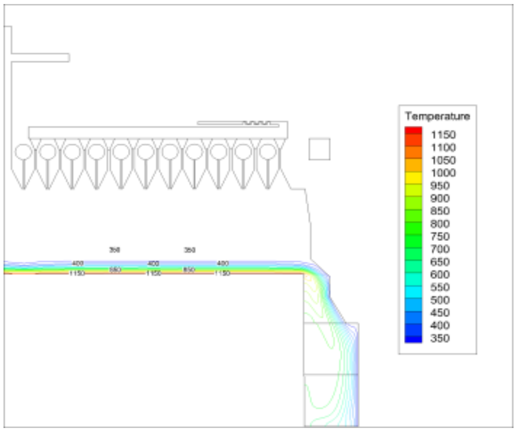
(d) 300 torr

Figure 12 The vector diagrams under different operating pressures

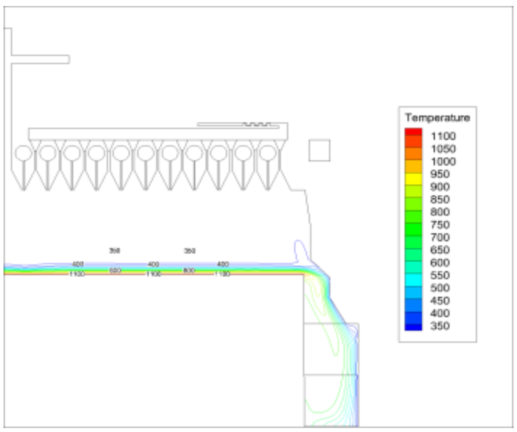
As shown in **Figure 13**, the change of gas flow is caused by pressure change, it also has some influence on temperature layer on substrate surface. With the increase of pressure, the temperature layer becomes steeper due to the influence of heat buoyancy which caused by the reduction of density. The high-temperature region is substantially parallel to the surface of graphite susceptor, and temperature distribution is uniform, which is conducive to the growth of material. With the increase of rotation speed of susceptor, the temperature difference near the surface increases, but the high-temperature layer thickness decreases, which may due to the axial pumping action caused by the rotation of susceptor, so that temperature distribution on the susceptor surface gets more stable. But in the case of high operating pressure, change of the vortex caused the change of gas flow in reactor, making it easy to cause the wall reaction.



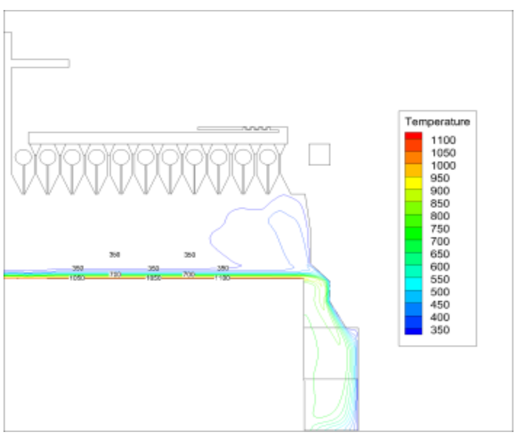
(a) 100 torr



(b) 150 torr



(c) 200 torr



(d) 300 torr

Figure 13 The temperature contours under different operating pressures

As shown in **Figure 14** is the substrate deposition rate distribution trend and film deposition rate with operating pressure increases. With the increase in operating pressure of the deposition rate also increases, which is consistent with the literature [20]. As shown in **Figure 15**, average deposition rate increases with pressure increase, when pressure is low, transmission rate increases with the increase of diffusion coefficient, which is helpful to the rapid diffusion of reactant molecules, and it can also weaken the disadvantage of the reactant molecules non-uniform composition distribution at atmospheric pressure.But if pressure is too low, the gas flow rate will be very large, most of the reactant will be discharged from the pump that consumption of raw materials increase, and the gas density becomes very small, thereby the deposition rate decrease. It also appears that the uniformity of deposition rate increase gradually, and the increase rate is gentle. When operating pressure is 300torr, the variation coefficient is less than 5%.

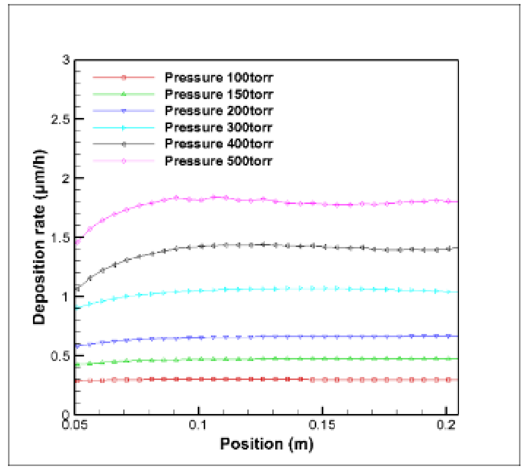


Figure 14 Deposition rate distribution on the substrate surface under different operating pressures

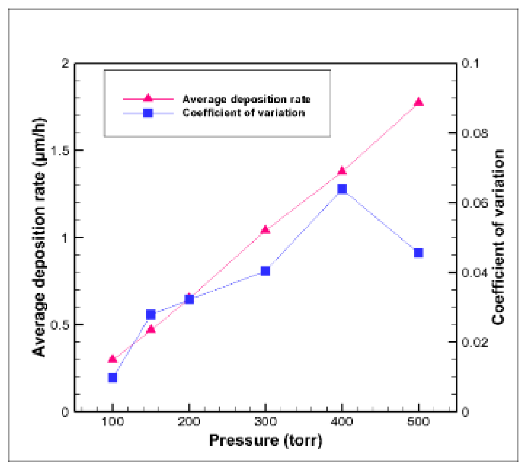


Figure 15 Average deposition rate and coefficient of variation under different operating pressure

6. CONCLUSION

In this paper, computational fluid dynamics software is used for three-dimensional simulation and research on the vertical-spray GaN-MOCVD reactor. Effects of process parameters which adjust within a certain range on flow field and temperature field in the reactor are discussed, and the operating parameters are optimized. The main results obtained are as follows:

(1) Increase in flow rate is conducive to the stability of flow field in reactor, but there is not a multiple increase in

average deposition rate of thin film, and there will be some improvement in the uniformity of deposition rate. But when the flow rate is larger, the flow rate fluctuation is more obvious, and the uniformity of thin film will be reduced.

(2) Increase in rotation speed of substrate benefits for high average growth rate and uniformity of thin film, but it will have some impacts on the stability of flow field. The higher the rotational speed, the more obvious rotating vortex will be.

(3) Increase in pressure is also beneficial to the average growth rate of thin film, but it will also have some impact on the stability of flow field and the uniformity of thin film. The higher operating pressure, the more obvious rotating vortex will be.

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