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Three-dimensional Simulation and Analysis of Spray Structure inVertical MOCVD Reaction Chamber

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Abstract: In the vertical spray MOCVD reactor, a spray structure composed of fan bodies was proposed. CFD was used to simulate the gas deposition process in GaN-MOCVD reactor. The characteristics of changing the concentration of reaction gas above the substrate surface with the height of the fan, the distance between the spray nozzle and the substrate surface, and the substrate rotation speed were given. Compared with the traditional spray structure, the cylindrical spray structure composed of fan body can effectively reduce the premixing problem of reaction gas sprayed from the spray nozzle before entering the reaction chamber and reaching the substrate surface. At the same time, the simulation structure shows that when other conditions are fixed, with the increase of the fan height, the increase of the distance between the spray nozzle and the substrate surface and the acceleration of the substrate rotation speed, the uniformity of GaN deposition on the substrate surface can be better under the same isolation effect, so that the utilization rate of TMG can be as high as possible under the condition that the uniformity is satisfied.

1.Introduction

Gallium nitride (GaN)-based semiconductor materials are one of the most important wide-bandgap semiconductor materials [1], and Metal-organic Chemical Vapor Deposition (MOCVD) is the key technology for preparing GaN films [2-3],generally use trimethyl gallium ($Ga(CH_3)_3$ referred to as TMG) and ammonia (NH_3) as Ga source and N source respectively, hydrogen and nitrogen as carrier gas, the optimum temperature for growth is about 1050 ℃[4- 5], because the group III TMG and the group V NH_3 must be mixed before reaching the substrate, a series of gas phase parasitic reactions occur in the reaction chamber to generate harmful nanoparticles, which are deposited on the inlet and outlet of the reactor and the upper wall of the reactor. It not only wastes precious source gas, causes the film quality to decline, but also makes the growth rate temperature, V/III ratio and other parameters change drastically [6]. Studying the gas phase distribution in the reaction chamber and then reducing the pre-mixing of Group III TMG and Group V NH_3 are essential for reducing the parasitic reaction of the reaction gas in the reaction chamber and the uniformity of film growth, as well as the growth of high-quality GaN thin film devices.

In the past 20 years, researchers have carried out a lot of theoretical analysis and improvement on the horizontal reactor structure [7-9]. Yang et al. [10] compared the traditional horizontal reactor with the separated inlet horizontal reactor through experiments, and believed that the quality of the GaN film grown in the separated inlet reactor was better; Hardtdegen et al. [7] used experimental and simulation methods to compare the divided horizontal reactor has been studied, and it is believed that the divided inlet reactor can reduce the parasitic reaction and increase the growth rate of the film. In order to maximize the use of source gas and improve the quality of the grown film, this paper proposes a new type of spray structure. Through numerical simulation, appropriate device parameters are given.

2.Numerical simulation process of flow field in MOCVD reaction chamber

2.1. Spray structure and simulation model in the reaction chamber

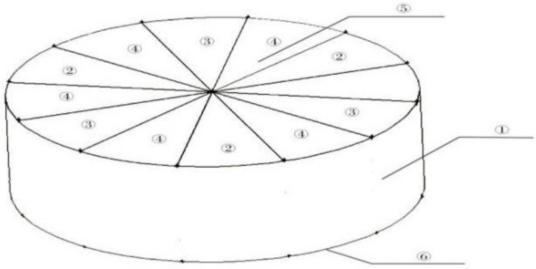


Figure 1. Schematic diagram of spray structure of MOCVD reaction chamber

Figure 1 shows a schematic diagram of the spray structure of the MOCVD reaction chamber. The device is composed of a cylinder, which is divided into multiple sectors. The sector (2) is the first gas channel participating in the reaction, and the sector (3) is Isolate the gas channel, the second gas channel where the sector (4) participates in the reaction. The sector surfaces of the sectors on the upper surface of the cylinder (5) are gas inlets, and the sector faces of the sectors on the lower surface of the cylinder (6) corresponding to the upper surface are gas outlets.

The reaction chamber is a cylindrical structure as a whole, in which the spray structure is a cylindrical structure composed of sectors. The central angle of each sector constituting the spray structure is 30. The gas flows in through the air inlet and flows through the sector. The spray port at the bottom of the sector flows out, and the radius of the spray device is equivalent to that of the base, which is 232.5mm. During the growth process, the base and the substrate are in a rotating state, and the speed is 500 to 2000 rpm.

2.2.Data simulation process and experimental method

This paper mainly studies the flow field in the reaction chamber and the concentration distribution of the concentration of the reactant gas on the surface of the substrate with the reaction conditions and the geometry of the reaction chamber. The hydrodynamic characteristics of the gas in the MOCVD reactor satisfy the mass conservation equation and momentum conservation equation. Energy conservation equation and composition conservation equation [10]. Therefore, the following assumptions are made without affecting the main simulation results:

(1) The gas is an incompressible, continuous fluid

(2) Regardless of the chemical reaction between particles, only the convection and diffusion effects between TMG, NH3 and H2 are considered;

(3) Numerical simulation ignores thermal radiation;

(4) The base temperature is regarded as a fixed temperature;

(5) The outer wall can be regarded as isothermal or adiabatic conditions;

(6) All walls in contact between the fluid and the reaction chamber adopt no-slip boundary conditions;

Based on the above premise, use gambit software to build a three-dimensional model of the MOCVD reaction chamber.

In order to be closer to the actual situation, in the simulation process, the same parameters as the actual are selected as the reference conditions: the central angle of the sector is always 30°, the base radius is 232.5 mm, the height is 2mm, and the reaction chamber radius is 242.5 mm, the gas inlet radius r = 232.5 mm. The main reaction gases in the simulation process are TMG and ammonia (NH3), the carrier gas is hydrogen (H2), the V/III ratio is 1000, the mass fraction of TMG is 0.029, and the gas inlet flow rate is v = 0.5 m/s, The acceleration of gravity g = 9.8 m2 /s, the surface temperature of the base and the substrate is constant 1050℃, the temperature Tw of the wall surface of the reaction chamber is constant temperature 300 K, the gas temperature at the inlet and the gas outlet are both 300 K, and the pressure P = 1 atm. After the geometric model is established, appropriate structural meshing is performed on the overall 3D model, and finally the boundary conditions are given for calculation.

To verify the accuracy of the simulation results, the boundary conditions used in the numerical calculation are as follows:

(1) Inlet: Adopt the specified velocity boundary condition, that is, the velocity value, temperature and concentration value of the reaction gas at the given inlet;

(2) Gas outlet: Adopt the pressure boundary condition, set the pressure as a constant, and the normal guide number of other physical quantities at the outlet interface is 0;

(3) Wall surface: The wall surface temperature is given, and the speed is set as a non-slip boundary condition;

Using the controlled variable method, after setting the data in 2.2.1, set several groups of different spray nozzles to the substrate distances for MOCVD respectively, and then select the best conditions after obtaining the rules, then set different sector heights, and again according to the law, the optimal conditions are obtained, and the above data models are combined to study the influence of different substrate speeds on the flow field of the reaction chamber. After a certain simulation time, the simulation process finally converges, and 12 sets of simulation data under different conditions are obtained. Then, in order to facilitate the analysis, sample and analyze the vertical section of the reaction chamber at 0.5mm, 5mm, 10mm above the substrate and obtain the flow field distribution of TMG and NH3. Observe whether the premixing phenomenon is serious and whether the concentration distribution above the substrate homogenize and observe whether there is a vortex in the reaction chamber.

3. Analysis and discussion of simulation results

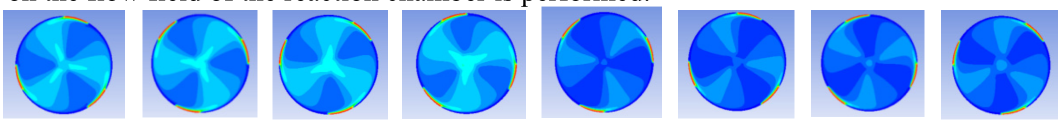
The key to the MOCVD epitaxial growth technology is to not only ensure the uniformity of the GaN film composition, but also deposit as much material as possible on the substrate to increase the growth rate. The following is a detailed study of the effects of the height change from the spray nozzle to the substrate, the height change of the sector, and the change of the substrate speed in the simulation analysis and experimental results on the flow field of the reaction chamber and the uniformity and concentration of the GaN composition above the substrate. In order to obtain the process parameters or reactor structure conducive to achieving high-quality epitaxial growth.

3.1.The influence of different sector heights (h1) on the flow field of the reaction chamber

Table 1 Simulation conditions for different sector heights (h1)

TMG sector angle	30	NH_3 sector angle	30	H_2 sector angle	30
TMG speed(m/s)	0.5	NH_3 speed(m/s)	0.5	H_2 speed(m/s)	0.5
The height of the sector h1(mm)	changes	The distance from the spray port to the substrate h2(mm)	30	The distance from the substrate to the air outlet (mm)	2
Substrate temperature (K)	1323	wall temperature(K)	300	Substrate speed(rpm)	1000
TMG：nh3	1000：1				

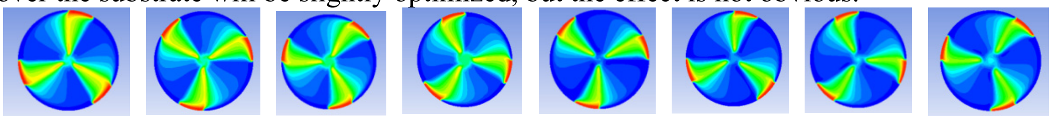
Table 1 is the setting of the data that is not changed when the simulation of the influence of the fan height on the flow field of the reaction chamber is performed.



(a) h1=20mm NH_3 (b) h1=30mm NH_3 (c) h1=40mm NH_3 (d) h1=50mm NH_3 (e)h1=20mm TMG (f) h1=30mm TMG (g) h1=30mm TMG (h) h1=40mm TMG

Figure 2. Streamline diagram of flow field distribution of GaN composition at 0.5mm above the substrate under different sector heights (h1)

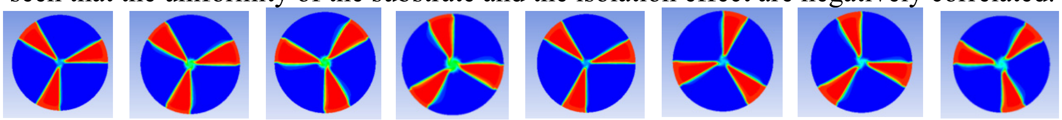
Figure 2 respectively represents the flow field distribution streamlines of the GaN components (TMG and NH3) at the height of the sector (h1) 0.5mm above the substrate. It can be seen from the figure that as the height of the sector increases, the uniformity of the GaN composition (TMG and NH3) over the substrate will be slightly optimized, but the effect is not obvious.



(a) h1=20mm NH_3 (b) h1=30mm NH_3 (c) h1=40mm NH_3 (d) h1=50mm NH_3 (e) h2=20mm TMG (f) h2=30mm TMG (g) h2=30mm TMG (h)h2=40mm TMG

Figure 3. Streamline diagram of the flow field distribution of the GaN composition at 5mm above the substrate at different heights (h1) from the nozzle to the substrate

Figure 3 respectively represents the flow field distribution streamline diagrams of the GaN components (TMG and NH3) at 5mm above the substrate under different sector heights (h1). It can be seen from the figure that the susceptor and the substrate are rotating, causing the gas above the substrate to drift laterally. As the height of the sector increases, the same initial velocity of the air inlet will reach the top of the substrate. The component speed will become smaller, so the lateral drift phenomenon will be more serious, so that the isolation effect of the GaN component (TMG and NH3) above the substrate will be worse, that is, the mixing phenomenon of TMG and NH3 will be more obvious (here can be Observe the overlap between the two sets of images to indicate the mixing of the two components), resulting in a small amount of parasitic reactions. By combining it with Figure 2, it can be seen that the uniformity of the substrate and the isolation effect are negatively correlated.



(a) h1=20mm NH_3 (b) h1=30mm NH_3 (c) h1=40mm NH_3 (d) h1=50mm NH_3 (e) h2=20mm TMG (f)h2=30mm TMG (g)h2=30mm TMG (h) h2=40mm TMG

Figure 4. Streamline diagram of the flow field distribution of the GaN composition at 10mm above the substrate at different heights (h1) from the nozzle to the substrate

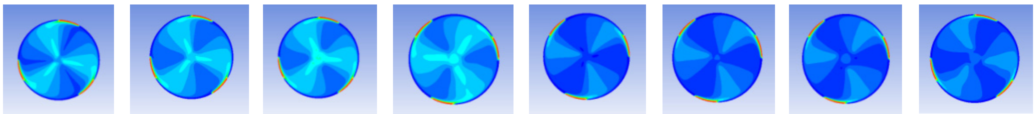
Figure 4 respectively represents the flow field distribution streamline diagrams of the GaN components (TMG and NH3) 10mm above the substrate under different heights (h1) from the spray port to the substrate. It can be seen from the figure that at 10mm above the substrate, the isolation effect of TMG and NH3 components is good. By observing the simulation data, it is found that only a small amount of TMG and NH3 components will be mixed at 8mm above the substrate (the data is taken from h1=50mm), which proves that the equipment performance can greatly reduce the parasitic in the reaction chamber reaction.

3.2.The effect of the height (h2) from the spray nozzle to the substrate on the flow field of the reaction chamber

Table 2 is the setting of the data that is not changed when the simulation of the effect of the height from the spray port to the substrate (h2) on the flow field of the reaction chamber is performed.

Table 2 Simulation conditions for different heights (h2) from the spray port to the substrate.

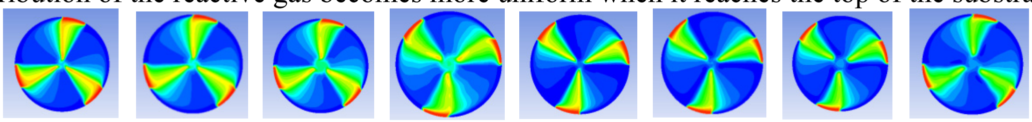
TMG sector angle	30	NH_3 sector angle	30	H_2 sector angle	30
TMG speed(m/s)	0.5	NH_3 speed(m/s)	0.5	H_2 speed(m/s)	0.5
The height of the sector h1(mm)	20	The distance from the spray port to the substrate h2(mm)	chan ges	The distance from the substrate to the air outlet (mm)	2
Substrate temperature (K)	1323	wall temperature(K)	300	Substrate speed(rpm)	100 0
TMG：nh3	1000：1				



(a) h2=20mm NH_3 (b) h2=30mm NH_3 (c) h2=40mm NH_3 (d) h2=50mm NH_3 (e)h2=20mm TMG (f) h2=30mm TMG (g) h2=30mm TMG (h) h2=40mm TMG

Figure 5. Streamline diagram of the flow field distribution of GaN composition at 0.5mm above the substrate at different heights from the spray port to the substrate (h2)

Figure 5 represents the flow field distribution streamline diagrams of the GaN components (TMG and NH3) at 0.5mm above the substrate at different heights (h2) from the nozzle to the substrate. It can be seen from the figure that as the distance from the spray port to the surface of the substrate increases, the distribution of the reactive gas becomes more uniform when it reaches the top of the substrate.



(a) h2=20mm NH_3 (b) h2=30mm NH_3 (c) h2=40mm NH_3 (d) h2=50mm NH_3 (e) h2=20mm TMG (f) h2=30mm TMG (g)h2=30mm TMG (h) h2=40mm TMG

Figure 6. Streamline diagram of the flow field distribution of the GaN composition at 5mm above the substrate under different heights (h2) from the nozzle to the substrate

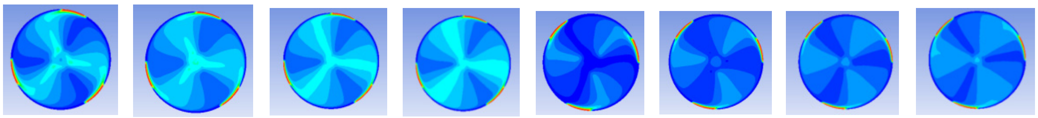
Figure 6 respectively represents the flow field distribution streamline diagrams of the GaN components (TMG and NH3) at the height of the substrate (h2) from different spray ports to the substrate 5mm above the substrate. It can be seen from the figure that as the distance from the spray port to the substrate surface (h2) increases, the velocity of the gas when it reaches the top of the substrate decreases. The smaller the velocity, the more serious the drift phenomenon and the worse the gas isolation effect. However, it is still obvious that TMG and NH3 are isolated from each other, and only a very small amount of parasitic reactions will occur. Observing the GaN composition (TMG and NH3) 10mm above the substrate, it is found that the gas is still in a completely isolated state. Only 8mm above the substrate (data taken from h2=50mm), there will be a small amount of mixing.

3.3.The influence of different substrate speeds on the flow field of the reaction chamber

Table 3 Simulation conditions at different substrate speeds

TMG sector angle	30	NH_3 sector angle	30	H_2 sector angle	30
TMG speed(m/s)	0.5	NH_3 speed(m/s)	0.5	H_2 speed(m/s)	0.5
The height of the sector h1(mm)	30	The distance from the spray port to the substrate h2(mm)	30	The distance from the substrate to the air outlet (mm)	2
Substrate temperature (K)	1323	wall temperature(K)	300	Substrate speed(rpm)	chang es
TMG：nh3	1000：1				

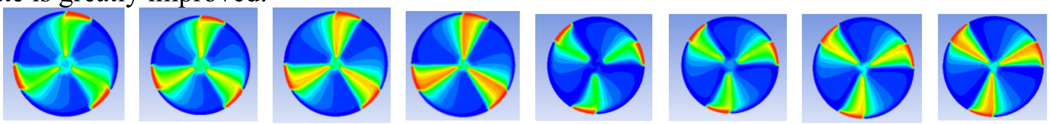
Table 3 is the setting of the data that does not change when the simulation of the influence of different substrate speeds on the flow field of the reaction chamber is performed.



(a) rpm=500 NH_3 (b) rpm=1000 NH_3 (c) rpm=1500 NH_3 (d) rpm=2000 NH_3 (e) rpm=500 TMG (f) rpm=1000 TMG (g) rpm=1500 TMG (h) rpm=2000 TMG

Figure 7. Streamline diagram of flow field distribution of GaN composition at 0.5mm above the substrate at different substrate speeds

Figure 7 respectively represents the flow field distribution streamlines of the GaN composition (TMG and NH3) at 0.5mm above the substrate at different substrate speeds. It can be seen from the figure that as the rotation speed of the substrate increases, the uniformity of the composition above the substrate is greatly improved.



(a) rpm=500 NH_3 (b) rpm=1000 NH_3 (c) rpm=1500 NH_3 (d)rpm=2000 NH_3 (e)rpm=500 TMG (f) rpm=1000 TMG (g) rpm=1500 TMG (h) rpm=2000 TMG

Figure 8. Streamline diagram of the flow field distribution of GaN composition at 5mm above the substrate under different substrate speeds

Figure 8 represents the flow field distribution streamline diagrams of the GaN components (TMG and NH3) at 5mm above the substrate under different substrate speeds. It can be seen from the figure that as the rotation speed of the substrate increases, the component drift phenomenon above the substrate decreases, and the gas isolation effect becomes better. It can be clearly seen that TMG and NH3 are isolated from each other, and only a very small amount of parasitic reactions will occur.

3.4.Distribution of longitudinal gas vector

All the above simulations can get the same lateral H2 velocity vector diagram, roughly as shown in Figure 9:

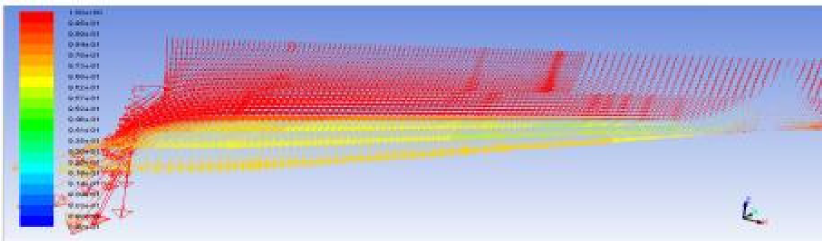


Figure 9. Axial cross-section velocity vector of H_2

It can be seen from Figure 9 that there is no vortex in the flow field, and gas transportation is ideal.

4.Conclusion

This paper is based on fluid dynamics (CFD) technology to simulate the three-dimensional space of a vertical spray MOCVD reaction chamber. The simulation results effectively reproduce the flow field structure of the GaN-MOCVD reaction chamber in the three-dimensional state. The reaction results have important reference value for achieving high-quality epitaxial growth process parameters and optimizing reactor structure:

Numerical simulation found:

(1) Changing the height of the sector has little effect on the flow field of the reaction chamber, and changing this parameter has little significance.

(2) By increasing the distance between the shower head and the substrate, the concentration distribution of the components above the substrate can be improved, but the isolation effect of different components will become worse. In general, the distance should be kept between 30mm-40mm Appropriate.

(3) By increasing the rotation speed of the substrate, it is very intuitive to see that the uniformity of

the components above the substrate becomes better, and there is still a good isolation effect before the components reach the substrate, but the rotation speed of the substrate cannot. If it is too large, the simulation results show that the speed of the substrate cannot be greater than 2000 rpm, otherwise the reaction results will not converge.

Acknowledgments
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