Numerical Evaluation of Growth Conditions of GaN-based LEDs in Multiwafer MOCVD Reactor

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ABSTRACT

In this paper, a novel super large metal organic chemical vapor deposition (MOCVD) reactor with three inlets located on the periphery of reactor was proposed and numerical evaluation of growth conditions for GaN thin film was characterized. In this design, the converging effects of gas flow in the radial direction could counterbalance the dissipation of metal oxide source. The growth of GaN films using TMGa as a precursor, hydrogen as carrier gas was investigated. For the mathematical solution of the fluid flow, temperature and concentration fields, the commercialized computational fluid dynamics (CFD) based solver-Ansys-FLUENT was utilized. A 2-D model utilizing axisymmetric mode to simulate the gas flow in a MOCVD has been developed. The effects of the temperature, mass fraction, and the total flow of carrier gas on the flow field, temperature field, and species distribution were analyzed and discussed. The numerical simulation results shows all the fields distribution were in an acceptable range.

Keywords: Numerical simulation, MOCVD, CFD, LED

1 INTRODUCTION

GaN-based blue light emitting diodes (LEDs), since first demonstrated by Shuji Nakamura, have been the hottest topic [1, 2] due to its great effect on full color display and solid state lighting industry. Many developments and novel technology have been used to improve the optical performance, thermal performance, reliability, and so on [3, 4]. The metal organic chemical vapor deposition (MOCVD), which is the fundamental assurance of the LED performance, is still the most widely used equipment for epitaxial growth of GaN. Currently, several limited commercial MOCVD models have been developed, including Axtron in Germany, Vecco in USA, Nippon Sanso and Nissin Electric in Japan, where the previous two types dominates more than 90% of the whole market and the products of the last two companies only existed in Japan. Intensive high technologies have been utilized to obtain good performance of reactor design, which is the heart of the MOCVD. However, there are inherent shortcomings [4, 5] in these products. For the vertical type MOCVD, the high rotating speed and close coupled showerhead brings complex design and low long-time reliability; for the radial type, the dissipation and depletion of metal oxide (MO) source in radial direction also leads to non uniformity of film, even if planetary rotating can counterbalance part of the dissipation effect, which also brings complexity of reactor design, water leakage in the showerhead, and so on. Besides, all of the currently existed reactors cannot be easily scaled up to a large scale without losing the uniformity and stability, which was required for the low cost and increasing demand for large yield [5, 6].

For the design of complex equipment like MOCVD, numerical simulation considering various process chamber configurations is very important to reduce the cost during research and development, save developing period, and insure the quality of equipment. Further more, experienced numerical simulation can also be used during the optimization of process [5, 6, 7, 8].

In this paper, the novel super large MOCVD reactor with three flows located on the periphery of reactor was proposed and numerical evaluation of growth conditions of GaN was characterized. The converging effects of gas flow in the radial direction could counterbalance the dissipation of metal oxide (MO). A two-dimensional model was put forward to study the performance of proposed MOCVD reactor. Feasibility of obtaining high quality GaN film by the novel design was studied numerically with various flow velocities and species.

2 NUMERICAL CALCULATION

In this work, a novel reactor design was proposed and characterized. Different from commercialized MOCVDs, three layers of circular slits located on the periphery of reactor were used as the three flow inlets for the novel reactor. The outlet was located at the center of the reactor. Details of the reactor design were shown in Fig.1. Comparing with conventional MOCVD, there are many advantages for this novel design. Firstly, for this design, the converging effects of gas flow in the radial direction could counterbalance the dissipation of MO source during the GaN deposition. Secondly, there isn't any complex component in the ceiling wall such as hole for gas inlet.

Simple design of ceiling wall means the thoroughly cleaning can be done in a reduced time and a simple process, where the uniformity, repeatability and reproducibility can be assured. Besides, specially designed spray board located between top and middle inlets was used to help obtain uniform flow distribution and sharp temperature gradient. From the the inset graph of Fig.1, it can be seen that the spray board was composed of two stainless steel plate with circular slits with coolinlg pipe located between them which can prevent the pre-reaction effectively by reducing of the nearby temperature. Furthermore, the spray board was designed to have one entrance and two exits which can ulteriorly improve the flow uniformity.

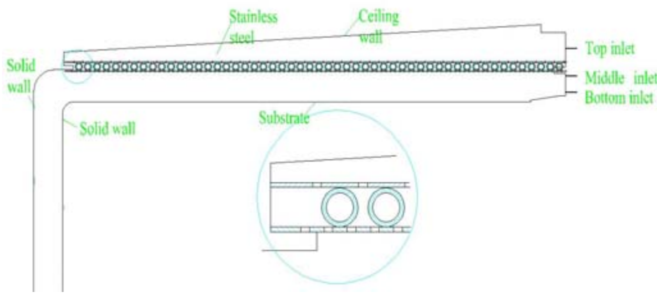


Fig.1 Schematic setup for the novel MOCVD reactor, The inset graph is an enlarged view of the spray board.

For the mathematical solution of the fluid flow, temperature and concentration fields, the commercialized computational fluid dynamics (CFD) based solver-Ansys-FLUENT was utilized. A 2-D model utilizing axisymmetric mode to simulate the gas flow in a MOCVD has been developed. The model takes into account the momentum conservation equation coupled with heat transfer and mass transport of the chemical species [6]. During the numerical calculation, following assumptions were made to simplify the complicated physical process: constant susceptor and wall temperature; neglecting of the radiation effect; chemical reactions are neglected; reactant concentrations are determined only by flow convection and molecular diffusion; Non-compressive ideal gas behavior is assumed. In order to insure the accuracy of the calculated results, convergence absolute criteria for energy and all the transported species was set to be 1e-6. The growth of GaN films using Trimethylgallium (TMGa) as the MO source, ammonia (NH_3) as the N source, and hydrogen (H_2) as carrier gas was investigated. It has been proven that the use of very detailed geometrical models is of crucial importance for accurate predictions [9, 10]. Therefore, no geometry simplification was made within the framework of the developed model.

3 RESULTS AND DISCUSSIONS

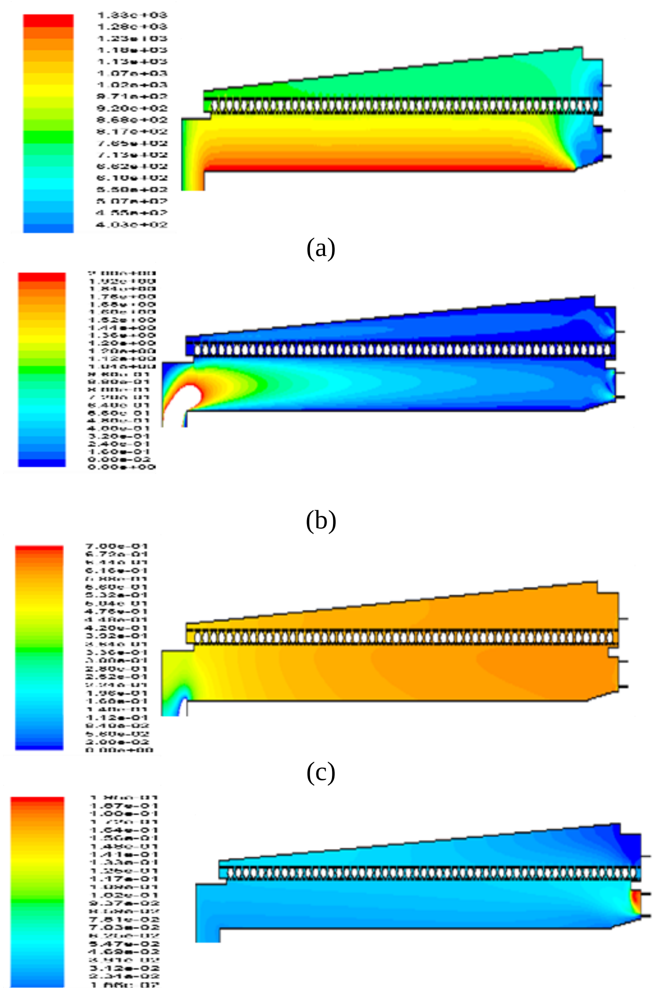
3.1 Effects of Flow Rates and Mass Fraction of Various Species

In order to verify the feasibility of the novel reactor, effects of various mass fractions of species and flow rates at the three inlets were investigated. The flow conditions for different cases were shown in table 1. Steady state simulation was used with the following boundary conditions: laminar model, pressure of 100 KPa, constant and uniform susceptor temperature of 1333 K, convection-determined temperature distribution, neglecting of radiation effect, inlet gas temperature of 300 K.

	Species	Case 1	Case 2	Case 3
Top inlet (SLM)	H_2	180	180	180
Middle inlet (SLM)	TMGa	0.7	0.7	0.7
	H_2	160.7	160.7	70.7
Bottom inlet (SLM)	NH_3	70	70	70
	H_2	90	0	0

Table 1 Species and corresponding ratio for the various flow conditions.

As a typical flow case, contours of calculated results for case 3 was shown in Fig.2 and the flow conditions in vector form at the slits on the spray board right after the inlets was shown in Fig.3.



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(d)

Fig.2 Simulation results for flow case 3: (a) Flow field (b) TMGa distribution (c) Static temperature field (d) Static pressure field.

From the flow field as shown in in Fig.2 (a), it can be seen that steady laminar flow right over the susceptor was obtained. No vortex or circulation occurred right over the susceptor and spray board. From the pressure field as shown in Fig.2 (b), it can be seen that the pressure above the spray board is higher than those areas below it, which means no back flow occurs on the slits of the spray board and the cross flow formed below the spray board would help to uniform the flow field. From the temperature field as shown in Fig.2 (c), it can be seen the temperature gradient is not too large in the horizontal direction right above the susceptor. And the temperature is low enough near the spray board and in the preheating area to effectively prevent the reaction. For the TMGa distribution, which is most important to the film deposition, is also uniformly distributed right above the susceptor as shown in Fig.2 (d), which means uniform film deposition speed and thickness.

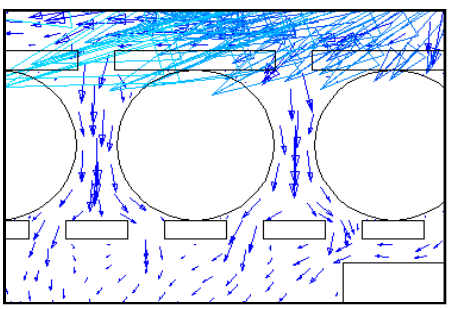

Fig.3 Flow conditions at the spray board right after the inlets.

As a typical demonstration of all the flow cases, it can be seen f rom Fig.3 that no back flows exist for all the flow cases, which is an evidence of the designed flow condition and guarantee of the efficient utilization of MO source.

It has been proved that the epitaxial growth rate of GaN thin film is dominated by the transport of TMGa to the susceptor [10], therefore the mass fraction of TMGa distribution right above the susceptor can reflect the deposition rate and the uniformity of the deposited thin films at the multi wafers in the radial direction. TMGa distribution on the susceptor was shown in Fig.4. From Fig.4, it can be seen for the case 1, 2, and 3, the increasing distribution of TMGa at the radial direction from inlet to exhaust were obtained. Fig.4 is kind of gratifying results to the epitaxial growth of GaN thin film, which means that gradually-increasing mass fraction of TMGa distribution can be obtained and the change rate can be modified by variation of mass flow and ratio of the composing species.

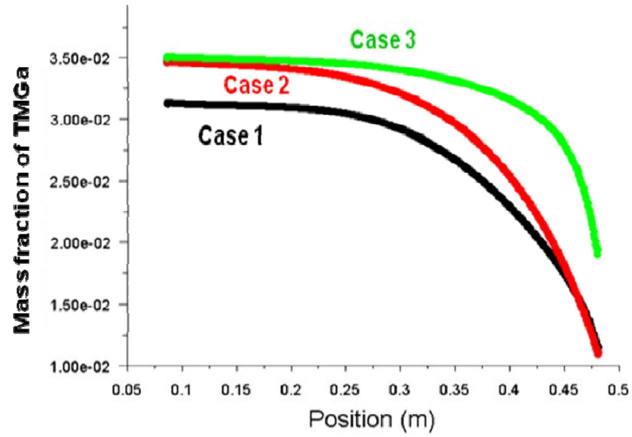

Fig. 4. TMGa distribution on the susceptor for flow case 1, 2, and 3.

Flow case 3 is the better one compared with the other two with the TMGa distribution increasing sharply at first and then change slowly, which means the use ratio of the susceptor is bigger. Combining the Fig.2, 3, and 4, we can say that even if with so large diameter (bigger than 1 m), high quality film could be assured from the novel designed MOCVD reactor in a near atmosphere vacuum degree. The novel design approach, using converging effect of the flow in the radial direction to counterbalance the dissipation of MO, was proved to be applicable.

3.2 Effects of Inlet Gas Temperature

In order to see the effects of the inlet gas temperature, same flow as case 3, 400 and 500 K were adopted as the temperature of inlet gas. The calculated TMGa distribution for inlet gas temperature of 300, 400, and 500 K were shown in Fig.5.

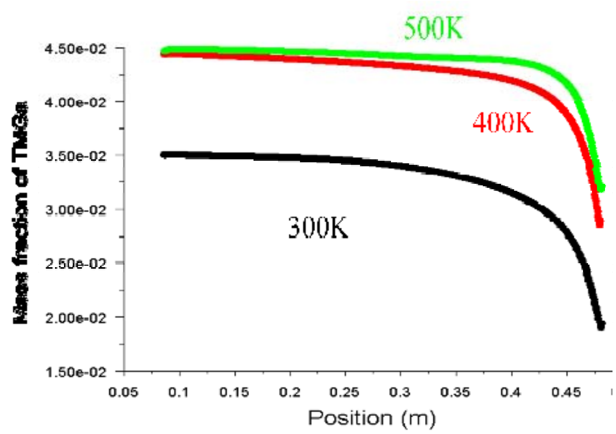

Fig. 5. TMGa distribution on the susceptor for inlet gas temperature of 300, 400, 500 K.

From the data demonstrated in Fig.5, it can be concluded that higher deposition rate of GaN and bigger use ratio of susceptor were expected when using higher temperature for inlet gas. However, increase of temperature for inlet gas could lead to higher temperature field for the whole reactor, which can cause the occurrence of pre-reaction in the chamber rather then only at the susceptor. The temperature distribution on the bottom of spray board was shown in Fig.6. Occurrence of pre-reactions in these zones not only affect the crystal quality of GaN but also lead to the cleaning and reliability problem for the reactor. Therefore, counterbalance between deposition rate and cleaning-reliability should be taken into consideration when making process design.

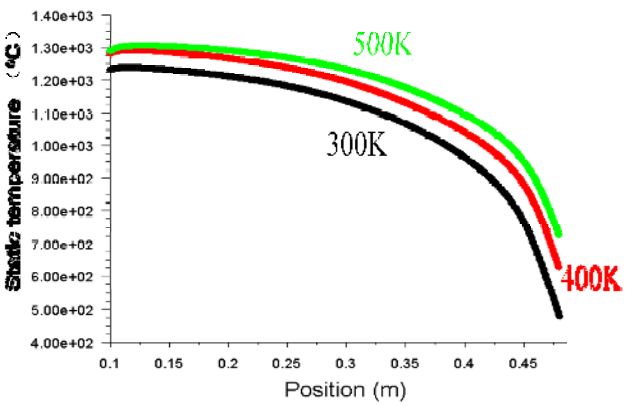

Fig. 6. Temperature distribution at the bottom of spray board for inlet gas temperature of 300, 400, 500 K.

4 CONCLUSION

In this paper, a multi wafer MOCVD reactor used for epitaxial growth of GaN-based LEDs with three layer circular flow was characterized. The numerical simulation results offer evidence for the potential high quality of GaN film by obtaining of laminar flow right over the susceptor, uniform temperature in the horizontal direction right above the susceptor and unirom TMGa distribution. In a word, the proposed novel design has been proved to own the ability to deposit uniform and high quality GaN film even in so large scale. And the fundamental numerical simulation offers reliable preliminary determination of experimental conditions and facilitate the optimization process of MOCVD design in a reduced time and cost.

5 ACKNOWLEDGEMENT

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