TECHNICAL PAPER

# Modeling and simulation of metal organic halide vapor phase epitaxy (MOHVPE) growth chamber

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Abstract Over the last few decades, there was a substantial appeal on the growth of gallium-nitride (Ga-N) based alloy for high performance optoelectronic devices such as blue/violet laser diode, blue/white light emitting diode etc. In the recent years, there have been revolutionary changes in semiconductor field. Growth method for GaN-based film has been extensively explored, with success of thick film growth using halide vapor-phase epitaxy technique. The theoretical changes were attributed from the experimental results where modeling was vastly used for the purpose of design of equipment. This is because of the cost of the equipment and it is one of the major burdens in semiconductor processing. This process constitutes an important technology for manufacturing thin solid film in the semiconductor industry. To address these issues, a new development called metal organic halide vapor phase epitaxy (MOHVPE) reactor has been proposed in this study. Modeling with five inlet nozzles with 54 cm long is designed by design software. The numerical study of horizontal MOH-VPE growth shows dependence on temperature and species flow rates. The inlet area is set to room temperature while the whole chamber is set in the temperature range from 1,273 to 1,473 K. Growth process reactor geometry that involved with temperature distribution stabilization and uniformity control flow pattern between the substrate holder are discussed. It is seen that the flow pattern

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is influenced more by the temperature distribution and geometry of the chamber. The numerical study of horizontal MOHVPE growth shows a function of temperature and species flow rates has been performed with specific condition to find the ideal position of the substrate for growth process in future.

## 1 Introduction

Nowadays, semiconductor industry move step ahead in development thin films (Narayan and Wang 2002). It developed the layers on the wafer to produce a semiconductor component. Metal Organic Chemical vapor deposition (MOCVD) of a thin single-crystal silicon film is growth on single-crystal silicon substrate of the same crystal-lographic orientation. While further perfected to growth thick layer of wafer is perform in halide vapor-phase epitaxy (HVPE) method. In both research and industrial field, Metal Organic Vapor Phase Epitaxy (MOVPE) has developed into a viable and necessary technique for production of semiconductor device layers. The epitaxial structure is the heart of the semiconductor device layer and MOVPE is considered the enabling technology for epitaxial growth of compound semiconductor devices.

Based on previous research, the insufficiency of this method which is MOVPE and HVPE are identified. Lack of uniformity wafer curvature produced caused by lattice mismatch that came from MOVPE method (Taiyo et al. 1998). Thermal expansion will affect the maximum crack occurs and nevertheless the threading dislocation will appear in minimum stage inside growth chamber (Taiyo et al. 1998). These happen when GaN was reacting with sapphire as substrate. Further improvement is carried out in HVPE method by using GaN to replace sapphire as substrate, after thin film has grown on the GaN as substrate, the process is continued by cutting the wafer into slice. This processed have to go through up to four instruments to get the results with refinement wafer or thin film. Later on, process of chemical mechanical polishing (CMP) to obtain uniformity is done. The final process is MOVPE growth to grow layers (combination of layers) for devices, such as light emitting diode (LED), laser diode (LD) and high electron mobility transistor (HEMT) proceed to get the surface uniformity of wafer in future experiments (Technology of Gallium Nitride 2005).

In conjunction with reactor design geometry and several identified inefficiency by experimental process, several studies have been focusing on developing the simulation tools aimed towards the optimizing flow pattern to produce uniformity. Currently, the design modelling for process method only involved in every single reactor has been brought forward which are MOVPE and HVPE methods of growth reactor. To address these issues, new development called metal organic halide vapour phase epitaxy (MOH-VPE) has been proposed. These are the hybridization between the growth reactor for MOVPE as well as HVPE concurrently in a single reactor.

The evolution of new design software was accustomed to design and simulate the process run by numerical analysis. Attention is paid to the growth of the chamber itself for analysing the reliability to withstand the heating process based on the simulation run. Both the Modelling as well as the simulation methodologies are discussed for such type of complex structure. Some significant issues i.e. controlling of the simulation and the material model are addressed. The applications for MOHVPE are illustrated in the presented analytical software for virtual product exploitation projects by software simulations.

The advantage of such system is the possibility to simultaneously growthick (high growth rate) and thin (low growth rate) GaN-based layer on a target substrate, without exchanging growth instruments when both thick and thin layer is necessary on the same substrate. Therefore, it reduces surface contamination, layer stress and substratebowing during cool-down and heat-up process, resulting samples with a lower threading dislocation density and higher film quality. While in having thin and thick film growth mechanisms coupled into a single growth reactor significantly simplifies growth preparation, during interreactor substrate transfer/steps and significant cost-reduction due to the procurement of less instrument/parts and with lesser maintenance. Researchers are mostly focusing on wafer growth uniformity without considering the effect of structure and geometry analysis flow pattern for mechanical analysis side (Utsumi et al. 2004).

This research opens the future on creative innovation and exploration in metal-organic and hydride gaseous

supply and control, thin and thick film growth techniques, electronic (HEMT) and optoelectronic (LED/LD/PD) devices fabrication in semiconductor research future ahead. Deposition technology is very useful and essential application in the electronic device manufacturing in the industries, especially to fabricate the semiconductor devices which are completely dependent on it. Thin solid films are formed from the deposition of various materials' gaseous, vapour, liquid and solidus phases in the semiconductor device manufacturing industries (Meyyappan 2000). In general, the gaseous phases of the materials contribute to grow the Epitaxial films of semiconductors. These films develop the layers on the wafer to produce a semiconductor component. Industrial and technological revolution has been observed in last few years. Semiconductor devices are also following that evolution and even helping other technical advancements to evolve further. The theoretical enrichment of the semiconductor devices are contributed from both the experimental setups as well as from modelling of the equipment design analysis significantly. Modelling, analysis and development of new devices in the semiconductor industries are encouraged due to increased financial burden of expenditures related to the sophisticated and advanced experimental set up establishment. The evolution of new equipment can often be achieved through trial and error procedure from the experimental set up utilization which is both time consuming as well as expensive, too. But this equipment design can be process optimized, efficient, less time consuming and less experimental work demanding once a reliable modelling is built. The models are accepted after effective validation process and then the model can be utilized for more parametric analysis to establish knowledge based technology for the process variables against their performances. For further observation on how the modelling can contribute, simulation consideration is needed to evaluate in initial stage of semiconductor process. First principles model may be further classified into analytical models and numerical or computational models based on how the equations comprising the model are solved. The complexities in the geometries of the semiconductor process simulations are the key obstacles in modelling the fabrication processes of semiconductor devices like transistors, led, etc.which are the branches of automation design for electronics, and the part of its one of the sub-field is known as technology CAD (TCAD). Previous research is conduct by hardware experimental setup to develop the wafer crystal growth and the main gases use is GaN. There is a considerable interest of Gallium Nitride for its broad band gapping and applications in the higher temperature electronics. From experimental hardware setups are successfully developed in the simulation setup for a reliable technology development recently. Researchers are focusing on the issues of improving the design geometry of the reactors and optimize the flow pattern uniformity into the reactors. Fluid flow models within both the horizontal as well as the vertical flow type MOVPE reactors have been published in several articles elaborately. Till now, only overviews of the previous processes which are MOVPE and HVPE growth reactors have been brought into forward. The HVPE method, defined as the potential growth technique so that both the large size as well as the thick crystal layers of GaN can be furnished (Zhao 2005). This is related to the fact that by this method, high growth rate is determined by mass input rate. It will cause melting of gallium through reaction of GaN at high temperature and near equilibrium process. While MOCVD process, produce lower growth rate with NH<sub>2</sub> in precisely controlled ambient temperature and pressure. This method is non-equilibrium process and it is suitable for growth of device graded thin film. Instead of high expenses between MOCVD and HVPE processes in different chambers, it is possible to concurrently grow thick and thin base layers on target substrates and reduced surface contaminants. To address these issues, new development called MOHVPE has been proposed. These are the results of hybridization between the growth reactor for MOVPE and HVPE simultaneously.

## 2 Growth chamber modeling

Based on the findings from the literature review, the design considerations of the growth chamber can be divided into few stages. Before describing those stages, it is to be mentioned that the initial point is to define the assessment method, i.e. which method would be considered as suitable design for the growth chamber of MOHVPE process based on the requirements or purposes. Based on the previous designs of MOVPE and HVPE reactors' specifications are identified for the new modelling of MOHVPE reactor having horizontal duct. This modelling of the reactor was performed in a computer aided software tool named SOLIDWORKS (Version 2011). The design was based on two dimensional (2D) and three dimensional (3D) models where atmospheric pressure was assumed inside the reactor in order to overcome the computational time. This design consists of five nozzle inlet with each of its 6 cm long arranged in 40 cm length horizontal direction with one outlet tube where the gasses dispenser as seen in Fig. 1.

There are 3 substrate holders which are used to observe the uniformity and to investigate the effect of geometry during the flow as shown in Fig. 2. The nozzle inlets are divided by long beam plate to prevent the mixing of gases before entering the chamber area as it is presented in Fig. 2.



Fig. 1 Modelling dimension of metal organic halide vapor phase epitaxy (MOHVPE) reactor



Fig. 2 Reactor modeling was performed based on 2D and 3D model with barrier between the inlet nozzles



Fig. 3 Inlet nozzles as the main entrance

#### **3** Nozzle inlet modelling

Nozzle inlet modeling in Fig. 3 is the major important part need to analyze for good expected as this chamber development with newly development as alternative for MOCVD and HVPE method. The main flow to consider is velocity and flow rate once pass by to enter the chamber and absorb wall will occur. Inlet velocity it is a common practice to design the inlet nozzle based on the momentum ( $\rho$ v2) of the entering fluid or air. The nozzle size depends on the presence of internals in the inlet nozzle. In every five single nozzle inlets inside the reactor, they are divided by long beam separation plates to prevent mixing of gases before entering the chamber area so they will meet shortly after the barrier passed by.

# 4 Simulation of flow pattern in MOHVPE growth chamber

The design of the chamber was used as the basis for FEM analysis, and its volume was divided into mesh elements in order to perform finite element analysis on its body. While creating the mesh of the chamber geometry, it is favourable to choose the mesh control, size of the element and their shape with global seed size is applied each part and element type is assigned. Mesh optimization process was performed to ensure the precision of the solver to obtain acceptable results. For an accurate result, a triangular mesh with a minimum element size 150 nm was used. Geometry of the chamber was solved using finite-element SolidWorks code 2011. Figure 4a, b shows the solution obtained using uniform meshing as obtained. Special attention has been appointed to capture the large fluctuations of the velocity in critical areas. But another type of mesh elements was obtained for the 3D geometries due to their design constraints. For this meshing representation, the studied region had more than 130,000.00(130K) elements.

The entire geometry of the reactor was not considered for the simulation owing to the rectangular symmetry; nevertheless, 2D simulation was not suitable for this case study. The inlets of  $H_2$  and  $N_2$  were dealt as the inflow boundary conditions presuming the flow of the gasses are laminar. NH<sub>3</sub> also flows through inlet 4 and 5 ranking from the bottom chamber. Hydrogen is heated up to 800 °C before starting the operation of the real system as there is a requirement of cleaning the full chamber to prevent the parasitic deposition. The gas is presumed as Newtonian in the continuum regime. Thermocouple was utilized to monitor the temperature from the centre of the wafer holder to maintain the growth temperature at set point.When the gasses get into the reactor up to required volume level, they reach at the temperature level same as the wall temperature which represents the furnace heating conditions.

The inlet flow velocity is set as a constant quantity of 0.05 m/s for all categories of simulations at each inlets. The temperature is varied between 1,273.2 and 1,473.2 K in all the simulations run. In the meantime, the pressure is set as 0.1 MPa for the opening of the pressure. Maintaining the heating system at every level is also necessitates due to risk of deposition of parasitic chlorides of ammonia. The chamber is divided into two zones with different





Fig. 4 Meshing generation geometry of Reactor chamber (a) Full body meshing (b) close up narrow inlet

**Fig. 5** Two zone area of temperature involved. (*I*) Inlet nozzle area (*II*) substrate holder area



Fig. 6 Middle holder is observed in simulation run

temperature. The inlets are extended towards the substrates as well as the temperature of the wall was set from 550 °C; the 5 inlet nozzles are set for flow under the room temperature of 27 °C for each inlet. While after pass the barrier the temperature in heat up between 1,200 and 1,000 °C as seen in Fig. 5. Central holder is stressed out to make clear of the best position for the required activities as observed in Fig. 6. Because of the crucial radioactive heat generations from the hot substrates, it was indispensable to make use of the corresponding models for heat transfer phenomena.

# 5 Analysis modeling

The simulation results can be utilized to determine the minimized among the substrate holder locations and observed the flow pattern surrounding the reactor geometry model. The results obtained in the calculation include flow patterns, reaction rate inside the chamber and volumetric flow since it also depends on presence of adsorbed layer at the chamber itself.

As discussed before, this is a novelty development while the result and the parameter involved in the real life applications is focused only on velocity and temperature influenced flow pattern with pressure constant inside the chamber. For the first stage, results were obtained with  $NH_3$  and outlets respectively located at 24 cm (1), 34 cm (2) and 44 cm (3) from the inlet nozzle to substrate holder is seen in Fig. 7 with the temperature profile. The system operates in such that both processes do not happen simultaneously, but first the system needs to be purged with nitrogen is set temperature 800 °C by vacuuming the chamber for three times with both MOVPE and HVPE before the gases start to enter. This is to make sure that the whole chamber is completely clean and free from dust and other pollutants.



Fig. 7 2D cross section view with 3 substrate holder allocated

# 6 Results

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Thus, the zone temperature was assigned after cleaning the inlet tubes preventing from getting muggy and tends to allow the gases to stick over the walls of the growth chamber. Flow through inlet duct typically is stable at the entrance of chamber but then the growth becomes rapidly faster after passing the inlet.

## 7 Geometry factor

Thermal decomposition due to reactions take place in reaction chambers thus generation of thin films experienced as desired output. The geometry of the reactor has significant influence on the flowing fluid's flow characteristics. Therefore, it is essentially regarded to optimize the reactor's shape to ensure smooth as well as laminar flow inside the chamber. The MOHVPE processes of the reactor posses several parameters that necessitate the careful design as well as optimization of the processes' parameters for effectively acceptable operation. Depending on the geometric factors for modelling, principal parameters which involve are the inlet area, the distance between the nozzles and the position of substrates' holders etc. critically prevent the recirculation in flow pattern. These critical parts are shown in the Fig. 8.

#### 8 Temperature effect surrounding the chamber

The temperature of the surrounding chamber is influenced by temperature of the chamber's body. The reactor is set to





control the temperature in a constant profile through reflex responses or changes (either raise or lower) as required. The main part of the geometrical effects with simulation analysis is based on up and down temperature rate surrounding it and would lead towards poor retention. Based on this phenomenon, the observation on temperature rate is analysed from 1,200 to 1,000 °C and it explained the three situations of temperature.

#### 9 Simulation result at 1,473 K

The simulation results with the inlet fluid temperature of 1,473 K (1,200 °C) could be observed in the Fig. 9. Here, the colour contour is showing the simulation model's temperature fluctuation at that given condition. The low temperature is indicated by the blue color then it will turned into light blue, green, yellow and at the end it is red

bution at 1,473 K

color indicating the high temperature band/contour in the regions. The simulation result is indicating the 5 inlet flows of fluid and air is under controlled temperature since it is set to be under room temperature. After a few iterations of the reaction chamber's interactive computation, the temperature appears to be rising through the lengthwise direction of the reaction chamber. After certain period of time the flow pattern grown up slowly to red color surrounding the chamber, It can be seen in the result where the contour of the color starts changing from red to yellow, green and last one is light green before it flows out of the tube outlets under the chamber itself to purge out all the unnecessary fluid at the end of the reaction chamber.

The result shows that the distribution of the temperature in reaction chamber seems decreasing at constant gradient. It could be visually perceived that the temperature distribution on substrate is not uniform and the temperature increase and turn to red chilis around the substrate after analysis on 1,273 K





passing the barrier at the nearly end of chamber. By definition of the red contour, it indicates that the critical areas along the three substrates are demonstrating well enough that 1,473 K is not suitable and could turn into dangerous cases if it is involved with the growth chamber later on.

#### 10 Simulation results at 1,373 K

Gas temperature features as well as the velocity characteristics obtained from the simulation results are investigated stage by stage for 1,373 K temperature. The red color contour is manifesting the high temperature, mainly at nozzle inlets and later changes into other quantified color contours till the lowest temperature. From the figures with color contours below, the red at inlet area indicating critically highest temperature while gas allowed into it. Once it passes, it will turn into light brown, yellow, green and light green at outlet area.

For the first stage as seen in Fig. 10, reaction of the gas flow can be assumed to be laminar and the temperature for the initial process is measured directly after gas flow is heated rapidly at inlet area. By the time the gasses enter the reactor, the gasses reached the temperature of the whole wall with no radioactive heat transfer incorporated in this chamber.

This condition occur because at the first gas nitrogen and NH<sub>3</sub> entered, it must be stable in certain time simultaneously while gas is heat up to stabilized back the environmental chamber. The mean flow velocity depends on the insulation diameter and their length through conductor wall. It was altered due to subject the liquid for different inlet flow. In a real case, the increased temperature might be varied alongside the axial position just after they are carried through the chamber for treatment.

# 11 Simulation results at 1,273 K

The results pointed out that the heating of the rapid gas is inside of the reactor's chamber system. The results obtained in this conceived calculations includes flow trajectory, rate of reaction inside of the reaction chamber. Temperature of the gases as well as their velocities is governed by the calculation.

After reaching at the subsector, the gas is heated up and the thermal entrance length needed for the gas to reach a fully developed temperature profile can be estimated roughly at 0.38 Re and at 1,273 K as in Fig. 11. As a result of heating up, vertical temperature and density gradients in the direction of gravity and perpendicular to the main flow direction are increased.

# 12 Analysis graph

Figure 12 shows the data for 1,473–1,273 K temperature distribution in the MOHVPE reaction chamber model versus different substrate position in three holders A, B and C. The profiles are normalized with respect from the inlet directly to the three holder substrate. The temperature for the III-V semiconductor material is defined at temperatures between 1,473 and 1,273 K. The first node at 1,473 K indicates the highest temperature along the chamber from inlet to the holder positions.





The second node 1,373 K situated at second highest temperature from inlet zone is strengthened by the optimum flow across distance to the end of chamber whereby it will flow directly without overspread before arriving uniformly inside the chamber. Based on growth itself, the wafer is easy to stick and difficult to remove from the holder which is too high temperature is tend to melt the growth in quick times. From the comparison among the range of temperature defined with based on simulation analysis, at node 1,273 K range is the most convenient area as observed at substrate holders positions with respect at between 35 cm distance from the inlet where the substrate B is located.

Based on these three temperatures and three different positions of substrate holders, the best optimum area to growth the layer and temperature is relied on 1,273 K at B holder. By taking into account the detail heat transfer in the process environment achieved an excellent temperature distribution. As mention before based on the profile plot, a good uniformity is observed in the middle substrate. Slowly down the temperature value from 1,273 K is the best performance flow once the gases enter with velocity 0.5 m/s to stable up the flow inside the chamber. The uniformity of temperature to growth up the wafer ranges from 1,273 to 1,050 K at B position (Fig. 12) clarified the best development of the wafer growth at middle holder.

# 13 Turbulent behaviour along the chamber

There are many thermodynamic as well as kinetic processes regarded in the growth reactions such that reactions in the system occur both homogeneously (gas phase) and heterogeneously (gas surface). In addition, reactor design must comply with basic hydrodynamic principles to reduce gas turbulence, allow for laminar flow of gas on the substrate and prevent competitive deposition on the chamber walls.

The Reynolds number at which the transition to turbulence occurs depends on the type of flow and area involved. Based on analysis computational simulation, Reynolds number which exceeds 3,000 proves that the flow is turbulent at inlet area nozzle, which is unstable flow. The validity of the observation is substantially dependent on iteration processes of both the turbulent and transient flows. None of the buffer layers were utilized at lower temperatures. The fluid flow in horizontal duct reactors can be very complex.

The turbulent flow occurred after the nozzle inlet and barrier area is only due to the fact that there is a potential to expose the mixing gaseous to unite with the temperature and gas entering the reactor flow. In the cold region at inlet nozzle, the flow rapidly develops to a laminar. Shorter reactor length reduces the turbulent effect with mixing zone that occurred inside the chamber in the inlet zone area and rapidly leads laminar flow surrounding the chamber as seen in Fig. 13 instead of reduce gas consumption. It is obvious from the flow pattern that reactive gases may turn in a circle and may change with the growth of parasitic at reactor walls.

Since the reactions mostly occur in the inlet nozzle, the barrier between each nozzle is one of the steps to avoid any flow mixing once the nitrogen and hydrogen enters as seen in Fig. 14 and reduced turbulent flow along the reactor. From these observations it can be seen that the high velocities and inlet mass flow reacts mostly at the inlet nozzle after the gas enters.

The design of efficient MOHVPE reactors requires adequate knowledge and careful observation in every stage of



Fig. 13 Turbulent occur at the inlet area after pass the barrier



Fig. 14 Turbulent flow that leads rapidly at inlet nozzle and becomes laminar surrounding the chamber

manufacturing and production processes. This needs to be considered before getting involved with the process system of growth chamber. It is evident from the results that temperature and gases consumption has been considered as rapidly consumed in the simulation analysis. The gas heating system is quite rapid inside of the reactor's model and thus gas consumption rate is in direct proportional to the heating requirement which influenced the modification of the geometric modelling. Since two distinct methodologies are involved within a single chamber reactor the geometric modelling should be meliorated for optimized performance.

# 14 Conclusion

A fundamental reaction of transport model gives the preliminary study showing the influence of the reactor geometry for two different processes in a single reactor. A newly developed horizontal flow single reactor MOHVPE has been conceived for design as well as simulation through utilization of 3D CFD-CAE modelling. This modelling of flow was run by simulation through SolidWorks Multiphysics Software based on modification of different parameters at each stage. Simulation results show that the performances inside the whole chamber of different geometries of the reactors can effectively influence the flow pattern with little effect on the uniformity of substrate holder.

The reactor's design ensures long-term stability and well defined mixing of gases on the substrate. By using the simulation developer, it can now design the mask shape for selective area. It is essential to optimize the reactor's design parameters to ensure thick layers film growth for semiconductor industries' exploration efforts of development. The importance of multiple reaction chemistry in horizontal growth at near atmospheric pressures and the strong interaction of gas flow with the deposition process in combination with relatively simple reactor geometry and the availability of large body seem to make this type or reactor very suitable for the evaluation comprehensive models.

The flow pattern of two phases flow in this simulation was observed through visualization. The patterns were identified based on literature study. While the superficial velocities of gases were adjusting, the transition of flow patterns could be observed. The observances indicated that the results from the simulation of flow pattern are obviously dominated by forcing gas convection owing to density variations of gas involved. Therefore, effective transportation to the substrates are achieved through careful selection of the carrier gases. It is evident that this is the best holder position to produce a uniform growth rate in this new development. It will reduce the worse uniformity profile for both processes by reducing time because predictions could be made by just running simulations.

Process simulations which are mainly performed to precisely project the distributions of active dopants and stresses as well as the geometry of the devices, too. This type of simulation is generally considered as the input for simulation of the devices, i.e. to model the electrical characteristics of the devices. The model gives logical results which relate very well with other researchers proved that MOHVPE model can be perfected with further investigation of the processes in the reactor for the next stage. It also assists to analyze the consequences of the alterations to the reactor's geometry by virtually developing those real time modelling events of actual physical reactors. Whereas, the real case could be time consuming. More investigations about the parametric changes indicate that little modification of reactor's geometry and substrates of the holders might lead to acquisition of acceptable uniform growth. Precise computation of the distribution of temperature parameter could be critical as the diffusion processes are fully affected by temperature. Therefore, such simulated modelling might be treated as beneficial to perform further optimum growth rates. New modelling of MOHVPE has established itself as the alternative to ease method of transferability of the process conditions among the key deciding factors and could be offered as a choice for planetary reactor for semiconductor industry capabilities.

The proposed instrumental setup for this research is a novel combination of both horizontal MOVPE/MOCVD and vertical HVPE. The considered research work opens future creative innovation/exploration in metal–organic and hydride gaseous supply/control, thin/thick film growth techniques, thin/thick film characterization techniques, electronic (HEMT) and optoelectronic (LED/LD/PD) devices fabrication and characterization methods, and standardization.

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