MODELING AND SIMULATION OF METAL ORGANIC HALIDE VAPOR PHASE EPITAXY GROWTH CHAMBER REACTOR

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FACULTY OF ENGINEERING
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MODELING AND SIMULATION OF METAL ORGANIC HALIDE VAPOR PHASE EPITAXY GROWTH CHAMBER REACTOR

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ORIGINAL LITERARY WORK DECLARATION

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Name of Degree: **MASTER OF ENGINEERING SCIENCE**

Title of Project Paper/Research Report/Dissertation/Thesis ("this Work"):

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Field of Study: **ENGINEERING DESIGN**

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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 (LD), blue/white light emitting diode (LED) 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 (HVPE) 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. In conjunction with reactor design, several studies have focused on the simulation for optimizing the flow pattern to produce uniformity in the system. To address these issues, a new development called metal organic halide vapor phase epitaxy (MOHVPE) reactor has been proposed in this study. The model is conjugated with comprehensive detailed simulation for horizontal tube reaction chamber by using computerized software. The development consists of 5 inlet nozzles with dimension of 54 cm long. The numerical study of horizontal MOHVPE 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 1273 K to 1473 K. Improvements of growth process reactor geometry aim that the velocity gas efficiency, temperature distribution stabilization and uniformity control flow pattern between the substrate holders are discussed. It is seen that the flow pattern is influenced 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.

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ABSTRAK

Selama beberapa dekad, terdapat banyak permintaan kepada pertumbuhan nitrid gallium berpangkalan aloi untuk alat-alat optoelektronik prestasi tinggi seperti biru/diod pancaran cahaya (LED) putih dan lain lain. Di tahun mendatang ini, sudah ada beberapa perubahan mendadak dlm bidang separa konduktor. Kaedah pertumbuhan untuk filem berasaskan GaN dengan meluas dijelajahi dengan kejayaan pertumbuhan ketebalan lapisan GaN dengan menggunakan teknik epitaksi fasa wap halide. Ini adalah disebabkan oleh kos peralatan dan ia adalah salah satu beban yang paling besar dlm industri semikonduktor. Dengan mewujudkan rekabentuk reaktor,beberapa kajian telah menumpukan pada simulasi kerana ingin mengoptimumkan corak aliran bagi menghasilkan keseragaman dalam system itu. Bagi menangani isu, satu perkembangan baru yang dikenali sebagai fasa wap halide organic logam reaktor epitaksi telah diperkenalkan dalam kajian ini. Model berkolaborasi dengan simulasi terperinci komprehensif untuk tindak balas tiub mengufuk dengan menggunakan perisian berkomputer. Pembangunan ini mengandungi 5 tiub laluan gas muncung dengan ukuran 54cm panjang. Kajian berangka pertumbuhan MOHVPE megufuk menunjukkan pergantungan pada kadar aliran suhu dan spesies. Luar salur masuk bersedia untuk dipanaskan pada suhu bilik manakala ruang proses tindak balas keseluruhan bermula dengan julat suhu dari 1273K hingga 1473K. Peningkatan geometri reaktor proses pertumbuhan adalah bertujuan untuk melihat kecekapan gas halaju yang masuk, penstabilan taburan suhu dan corak aliran kawalan keseragaman antara pemegang pertumbuhan GaN diperbincangkan, ia dilihat bahawa corak aliran dipengaruhi oleh taburan suhu dan bentuk geometri reaktor. Kajian berangka ini menunjukkan fungsi aliran suhu telah menunjukkan dengan keadaan unggul bagi proses pertumbuhan pada masa hadapan.

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CHAPTER 1 INTRODUCTION

1.1Background

Nowadays, semiconductor industry move step ahead in development thin films (Saridakis, et al.2008).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 crystallographic orientation. While further perfected to growth thick layer of wafer is perform in 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 react 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 slices. This process has 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 LED (Light Emitting Diode), LD (Laser Diode) and HEMT (High

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Electron Mobility Transistor) proceed to get the surface uniformity of wafer in future experiments (Gallium Nitride,et al. 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 (MOHVPE) 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 grow thick (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 substrate bowing 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

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preparation, during inter-reactor 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.

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.

1.2 Research Objective

The objectives of this research are:

1. Modelling and simulation a cost-effective chamber which capable of growing thin and thick layer thin film and alloys by using design software
2. To determine the effect of certain parameters on development a modelling chamber with computer simulation platform and optimization of these parameters.
3. To investigate the process flow influencing the reactor chamber at certain temperature and pressure.

1.3 Layout of Dissertation

This dissertation is outlined as follows:

Chapter 1Introduction

A brief background of the research, the research objectives as well as layout of thesis is presented in Chapter 1.

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Chapter 2 Literature review

Chapter 2 reviewed the state of art in this area of studies. A large number of recently published journal articles and theses is critically reviewed. In this chapter some relevant information are presented. The design of existing chamber and the technology behind that are covered and discussed. Some impact information is also included.

Chapter 3 Research Methodology

This chapter explains the detail of design modelling, parameters and simulation of growth chamber's settings. Analysis Simulation is run by software flow multi-physics SolidWorks co.

Chapter 4 Results and discussion

The data, results and discussions from investigation of growth chamber are Compiled and documented in Chapter 4.

Chapter 5 Conclusions and recommendations

This chapter consists of concluding remarks from the analysis performed based on the objectives of the thesis. Further recommendations are mentioned based on the knowledge achieved on this work, too.

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CHAPTER 2 LITERATURE REVIEW

2.1 THIN-FILM DEPOSITION PROCESSES AND TECHNOLOGIES

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 (Martin et al., 2009). 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. The process of deposition of chemical vapor of single-crystal silicon films on a substrate of single-crystal silicon with similar crystallographic orientation is known as homoepitaxy. The success of homoepitaxy development is governed by the diminution of hydrogen dichloro silane vapor. Deposition of thin films also can be considered for various other applications. Figure 2.1 (a) and (b) representing a type of generic thin film as well as the chamber to produce the thin films respectively for a typical application of thin film deposition

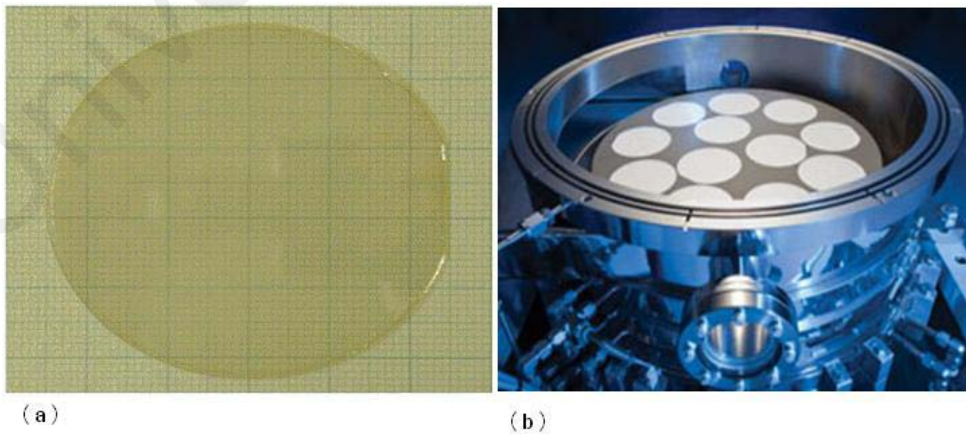

Figure2.1 (a) Thin film in semiconductor industry (b) growth chamber

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2.1.1 Modelling of Semiconductor Manufacturing Process

Industrial and technological revolutions have 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.

Semiconductor Manufacturing Networks process with good impact of economies worldwide (H. Mimura et al.1998). Fundamental knowledge of operation principle and effective technical applications of these devices govern the basis of their global enterprise extensively throughout such manufacturing networks. Otherwise, it will impossible for the engineers as well as for the decision makers to predict the acceptance of new manufacturing plant designs. One of the entries in Webster New Collegiate Dictionary for model is “to produce a representation or simulation of”. 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

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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).The type of modelling for Computational Fluid Dynamics & Multiphysics Solutions involved in the lead applications in extensive variety of multiphysics fields includes:

- Semiconductor industries include the plasma, deposition of chemical vapor simulations for semiconductors, medical technologies& solar industries.
- Energy: Analysis of thermal and structural performances for electrochemical devices like batteries and fuel cells. Automotive: Thermal management of vehicles, optimization of power train operations and thermal management, climate control & passenger thermal comfort, etc.
- Aerospace: aerodynamics in the higher& lower Mach number regimes.

Currently the sequenced famous processes those are used in the semiconductor industries is chemical vapor deposition (CVD) simulation and halide vapor phase epitaxial (HVPE). 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.

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2.2 MOCVD Fundamentals

Reactive gases pass over the silicon wafer in the MOCVD process. These gases are absorbed onto the wafer surface and react there thus form a film. This is one of the MOCVD reactor applications. When the products of the reaction leave the surface such as gases are pumped away, the reactions are reactivated either by thermal energy through heating the wafer or radio frequency (RF) energy through plasma (such as laser light are used). At typical MOCVD reactor system, the gases enter the chamber through inlet. They pass over the heated wafer then flow out the chamber to the pumps. Few MOCVD processes operate at atmospheric pressure due to the formation of gas phase particles. This is an essential process step in the manufacturing of microelectronic devices. High temperatures and low pressures are the most common process conditions, but are not necessary. All CVD involves using an energy source to break reactant gases into reactive species for deposition.

The basic principles of MOCVD are shown in figure 2.2.The Principles of a MOCVD-process are, (a) Laminar flow should be maintained for carrier gases (H2 or N2) and for the precursor molecules (i.e. compounds of metal-organic substances) throughout the substrates (wafer) by placing on a graphite susceptor in to the reaction vessel (reactor), (b) The thermal energy (generally ranges from 400°C to 700°C) should be supplied to decompose the molecules, (c) While the materials are under gone the deposition process, the molecular fragments are evaporated into the gaseous phases.

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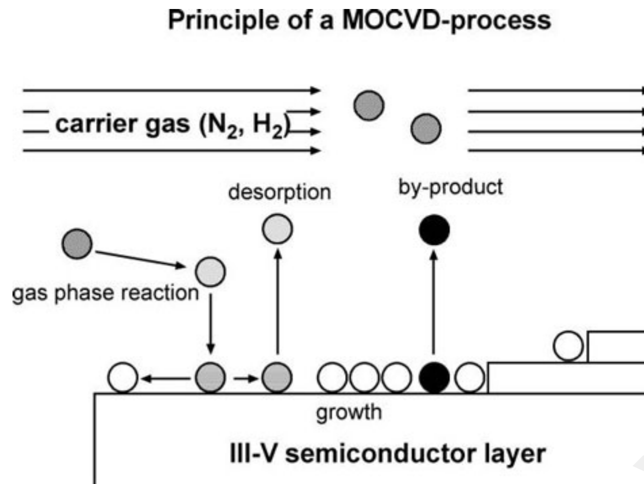

Figure 2.2 Principle of a MOCVD process
(Helmholtz Zentrum Berlin.co, 2006)

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The basic compound in semiconductor material that involves in MOCVD process is GaN. It shows tremendous potential in various applications of electronic as well as optoelectronic devices for few years because of its broader band gapping and higher collapsing/decomposing field properties (Z. Bandic et al. 1998). MOVPE process is considered as the main methodology to produce single crystalline layers of this compound material. Besides that, MOCVD provides the lowest cost and highest throughput of the two processes and it is more commonly used by the leading LED manufacturers for everything from traffic signals, car tail lights, billboards and signage to TV backlighting and general illumination (Bougrov et al.2001).

2.2.1 Specification of MOCVD Process

Chemical vapor deposition (CVD) is one of the widely used methods to deposit thin films of an extensively versatile range of materials. There are few phenomena observed in the MOCVD processes; coupled fluid flow, mechanism of heat transferring, mass transport of several gas species as well as the chemical reactions of gaseous phase and on the heated up substrates as seen in figure 2.3. In a typical CVD process,

chemical reactions take place to let the gaseous phase of the material compounds to deposit a thin film. At the room temperature, the gaseous reactants (which are frequently diluted in the carrier gas) enter in to the reaction chamber. The mixture of the gases is heated when it comes in contact with the surface of deposition, due to radioactive manner or being placed on a hot surface. Upon contingent of both the processes as well as the operating conditions, earlier to strike the surfaces the vapor phases of these reactant gases might be subjected to homogeneous type of chemical reactions. The boundary layers of thermal, momentum as well as the chemical concentration are formed when the stream of gases are heated, retards because of viscous drag and when there is any change in the chemical compositions. Deposited materials are formed at deposition surface when the source gases or the intermediary reactive species are undergone in to the Heterogeneous reactions. Finally, the by-products obtained in the reaction chamber due to gaseous reactions are carried out.

The main resources as precursor in MOCVD processes are used in growing epiwafers of III-V compounds. It uses metal organic compounds such as trimethyl gallium (TMG) or trimethyl aluminium(TMA) as precursors for the material in thin films. While as the process transports the precursors via a carrier gas to a hot zone (susceptor) within a growth chamber, thin films are produced when the precursors react or dissociate with another compound (http://www.veeco.com/metal-organic-vapor-phase-epitaxy.aspx). The growth chamber (reactor) is one of the places inside the experimental setup where the basic processes are occurred.

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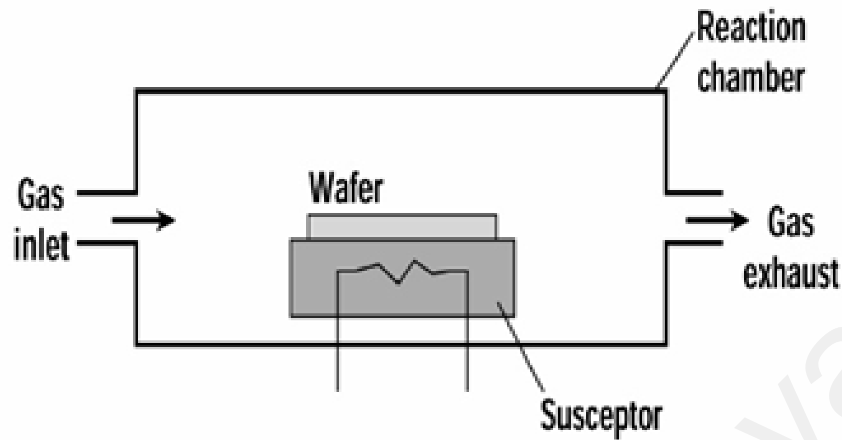

Figure 2.3 Basic Thermal CVD reactor (Veeco company, 2001)

It is essential requirement to have the knowledge about the mechanisms of the compound semiconductors that governs their growth rate. Thus, it renders both the suitable growth conditions and the insight into the crystal growth mechanism to prepare the compound semiconductors. There is an usefulness of equilibrium model to predict the rate of growth rate as well as the elements are incorporated of III–V compound semiconductors which are grown due of vapor phase epitaxy (VPE) along with metal

Organic vapor phase epitaxy (MOVPE), HVPE as well as the molecular beam epitaxy (MBE).It might be holding an attention to explore the intrinsic limits of growth rates of GaN compounds by MOCVD process. The recent evolution of GaN compounds based blue light emitting diodes (LEDs) and lasers (A. Barancco, et al. 2001)as well as the higher power/higher temperature electronic devices have contributed to a rapid active commotion of researches in the III-nitrides.

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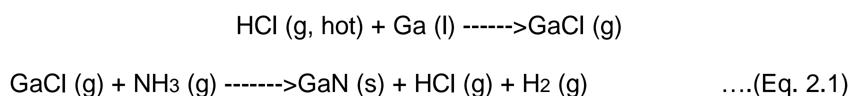
2.2.2 HVPE Alternative Method for MOCVD

MOCVD process is considered as the standard methodology to produce the thin GaN epilayers. Since this process has to be improved nowadays, therefore, Halide Vapor Phase Epitaxy is especially the common alternate to produce GaN samples (Craford.M.G, et al. 1997).

(Maruska and Tietjen, et al. 1969) first reported the hydride vapor phase epitaxy (HVPE) of GaN employing the substrates of sapphire (Holonyak Jr. N, et al. 1967) In the 1990s, HVPE growth of GaN drew attention to produce and prepare the freestanding up ofGaN wafers. HVPE process is an established atmospheric pressure, device growth process, where hydrogen chloride transport by hydrogen or nitrogen carrier gases, is passed over a source gallium nitride with support by sapphire wafer. Until the early 1980s the HVPE process had played an effective function as the singular available method to grow the epitaxial layers of GaN in the process of III-V semiconductor growth. Again in the 1990s, the HVPE had received keen interest due to its potential in growing thick films of GaN with lower defectiveness. In the HVPE process (equation 2.1), state the Group III nitrides (e.g., GaN, AlN) are produced through the reactions of hot gases of metal chlorides (e.g., GaCl or AlCl) by gas of ammonia (NH3). In this case, the hot HCl gas is passed over Group III hot metals to generate the chlorides of metals. The temperature inside of a quartz furnace is controlled well for all these reactions while the gas serves as carrier gas.



$$HCl\ (g,\ hot) + Ga\ (l) \text{------>} GaCl\ (g)$$

$$GaCl\ (g) + NH_3\ (g) \text{------->} GaN\ (s) + HCl\ (g) + H_2\ (g) \qquad \text{....(Eq. 2.1)}$$

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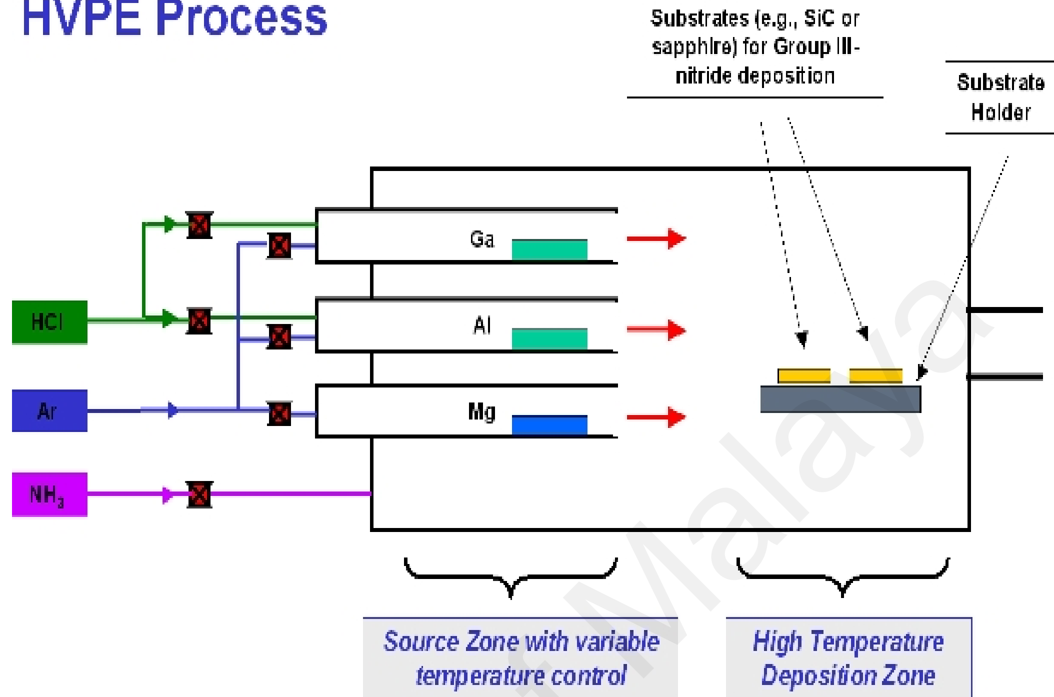

Figure 2.4 HVPE fundamental process (crystalFlex.co, 2002)

Metal Organic Chemical Vapour Deposition and HVPE have been well established since two decades ago. These processes constitute an important technology for manufacturing thin solids' film in the semiconductor industries. Currently, growth method for GaN based film has been extensively explored, with success of thick film growth using halide vapor-phase-phase epitaxy (HVPE) technique in figure 2.4. Device-grade crack-free thin-film growth was successful in 1986 using metal organic vapour phase epitaxy (MOCVD) by Amano Tech. and further perfected by (Nakamura, et al., 1998) using 2-flow MOVPE system. In many reactors HVPE design, the arrangement of inlet with different types is employed, to eliminate early mixing of reactants. However, problem defects such as reactor design itself must be encountered first as this is the main part to develop a good uniformity of wafer

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substrate. Based on previous developments, though there is already significant researches are performed on these materials the characteristics of the materials is far from perfection and there is significant amount of work being dedicated to ameliorate the characteristics of GaN. The advantages obtained from the HVPE processes since they are able to generate thick & highly toned Al GaN and AlN compounds to use in the optoelectronic as well as in the various devices of RF electronic. Unlike MOCVD, the HVPE processes not involve metal-organics and therefore, provide a 'carbon-free' environment for epitaxial growth.

2.3 Modelling Growth Process Chemical Vapour Deposition

Semiconductor materials have been studied intensively since the birth of silicon technology more than 50 years ago. The ability to physically and chemically tailor their properties with precision is the key factor which is responsible for the electronic revolution in our society over the past few decades. Semiconductor material systems (like silicon and GaAs-related materials) have matured at present and found their well established applications in electronics, optoelectronics and several other fields. There was a major upsurge in the research of the GaN material system around 1970.Several important developments in growth procedures in the mid to late1980s led to a resurgence and revival of the research interest in GaN and related materials. A method to grow smooth single crystalline GaN layers on a foreign substrate (i.e. heteroepitaxy on sapphire) using a thin (about 30 nm) low temperature grown AlN buffer layer was suggested by (Klaassen.D.B.M et al. 1992) This resulted in the rapid development and commercialization of III-Nitride light emitters (LEDs and lasers). For light emitting diodes, however, the advantages are not so obvious. Nevertheless, it is probably true that all GaN based devices would benefit in some respect from the reduced defect density possible from growth on high quality bulk GaN substrates. Hence, the

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development of suitable modelling growth techniques to produce bulk GaN substrates of high quality, at an affordable cost for commercial devices, has become a very important research area during the last decade.

Because of requirements there evolved various types of reactors and process design methodologies. Therefore, advantages could be obtained in further analysis of the reactors through this modelling analysis for considered reactor processes without any experimental modifications in the real reactor geometries. Based on the modelling analyses, the design of the reactors as well as the process variables' performances can be tracked with realistic boundary conditions and thus it can reduce the required trial and error in the experiments rather the experiments can be performed with particular focus as obtained in the accepted simulation results and therefore, both the time and cost can be optimized for better investment output. Technical evolution is also encouraged in this way.

2.3.1 GaN growth in Different Reactor Design

Generally, the thermal decomposition of the reactions (resulting in thin film deposition) takes place in the reactor chambers. Depending on the findings of the above mentioned analytical models, the geometry as well as the shapes of the reactors for high rate of growth and optimization can be achieved for excellent uniformity in the laminar as well as the vortex-free flows as can be seen in figure 2.5 below. It has been shown that the downstream flows can be melio rated if the susceptor size is increased.

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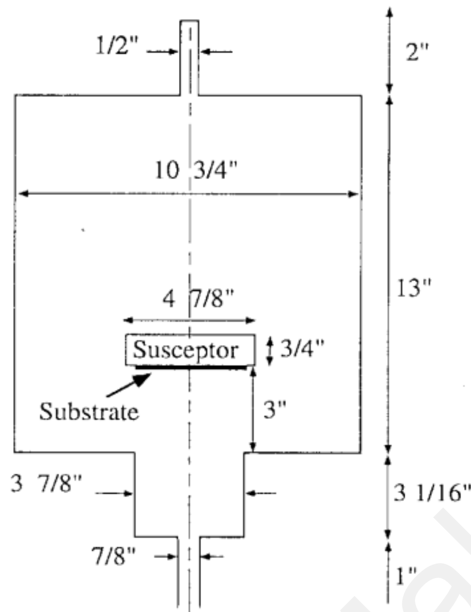

Figure 2.5 MOCVD reactor geometry (dimensions in inches)
(K.F Jensen, et al. 1996)

(Amano.H et al. 1969) stated that the geometry of the reactor chamber which was designed for the vortex of upstream flow is required to be removed as the reactor's dimensions as well as the shapes were changed. There is a requirement of heedful considerations while performing the optimization of the reactor in full range as the MOCVD operates throughout a broad scope of the experimental conditions. Inlet velocity of the gases is one of the most significant parameters to conceive. When the inlet velocities are high enough then the separation of the flow occurs on the reactor's walls. And therefore, there is a recommendation to increase the diameter of the reactor chamber's inlets so that there is a diminution of the gas velocity while maintaining constant mass flow rate. The reactor's geometry possesses considerable affect upon fluid flow features as (Mohammad.S.N et al. 2003) has stated that optimization of the reactor's shape is an essential consideration in assuring both the smooth as well as laminar flows (free from eddies) in the chamber. The investigation of GaN is proposed in two different methods and principle with variety of different reactor/chamber design

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geometry. The home-built experimental unit of GaN for reaction chambers are investigated. The reactor geometry is the important parameters during the uniformity of wafer growth. MOCVD process is one of the main methods employed to generate wafer of single crystalline layers from this material compound. At present, the gallium nitride device manufacturers are using both the commercial as well as custom built reactors' designs. (Rinku P. Parikh, et al. 2006) clarify that the wide range of reactor designs indicates a lack of a coherent framework on how to design GaN reactors for optimal single-wafer and multiple wafer production. As a result, Substantial exploratory research works have been taking place in both academic as well as industrial level which has raised the manufacturing technology in the past decade. (Nakamura.S, 1997) also stated that various reactor systems have been designed and developed by a lot of research groups worldwide, particularly the delivery systems of gas flow, with the mission to reduce the precursor interplays. It is worth mentioning that when these designs are about to be inhibiting these reactions in the delivery systems of gas flow. In this case, the precursors must completely mix to obtain the uniformity of the film thickness when it is very close to the wafer substrate. For this area, unequivocal realizations of both the physical as well as chemical mechanisms which govern the deposition processes do not even exist. The intricate intrinsically chemistry of the deposited ionic processes can be regarded as one of the difficulties in achieving such realization in some extent, the knowledge of which is Insubstantial till now. (Iwasa, N, and Nagahama, S, et al 1993) asserted that the quality of GaN films could be well improved through utilization of a reactor which should be especially designed by little modifications to their instrumentations to preclude the pre-reaction or generation of adducts. In conjunction with the designs of reactors, significant analyses led the focus on the evolution of simulation tools directed towards optimization of film thickness uniformity. Models are routinely utilized for optimization of designs and parameters of

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operation to generate thin films of GaN compounds with a spatial uniformity of thickness. Lately, a novel approach had evolved to control the uniformity for planetary CVD based pure geometries of the radial flows inside the reactors including the planetary rotation of the wafer. In MOCVD process, (Rinku P. Parikh, 1999) explicates that quality based prediction has been becoming more and more important for the generated film by different types of designs as well as the operation principles/ standards of the reactors.

2.3.2 Planetary Radial-flow Reactor Model Development

Efficient design of reactors for the growth chamber necessitates a consummate knowledge of chemical kinetics of the reactions occurred in the processes. The measures of the choices for reactor's operation principles and the design of their physics have a crucial influence on the property of being selective among various distinct reaction tracts, as in the cases of GaN compounds where two competing reaction tracts exist. Based on the published literary documents focus has been drawn on heedful designing of the delivery systems of gases for GaN based reactors with the objective of suppressing or avoiding the adduct in the pathways. A vertical cross- section of the radial flow planetary reactor system along with their physical domains is shown in figure 2.6. (Narayan.J et al. 2002) explicated that the precursors as well as the species of carrier gases are injected into the core of the reactor via a 2-flow type design for gas inlet and the flow to the outwards around the wafers which are arranged in the circular patterns over the susceptor. The design of 2-flow gas inlets allow group III compounds to be acquainted individually from the compounds of group V. In such reactors, the rotating satellites are arranged to put on the wafers which successively rotates about the central axis of the susceptor plates(as the planetary rotation). It is to be mentioned that

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reactors of such type could be operated with both the rotating and the stalled (non - rotating) wafers.

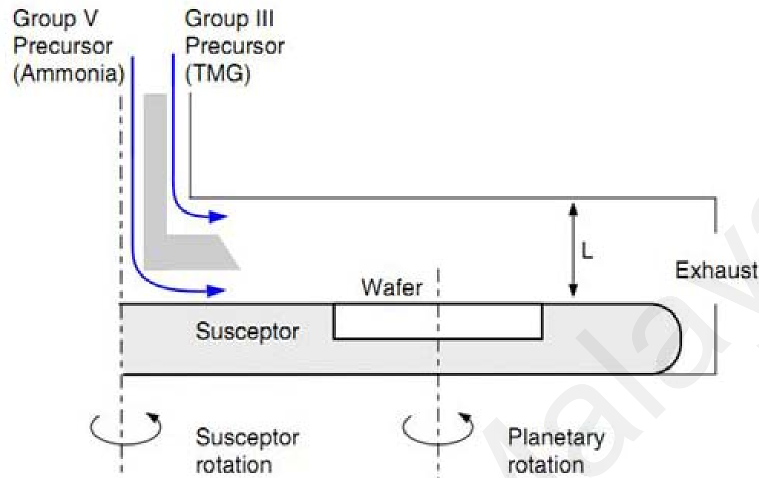

Figure 2.6 Vertical cross- sectional view for reactor geometry
(Rinku P. Parikh, 1999)

(Rinku P. Parikh, et al. 1999) pointed out from their research outputs that these pathways that took place are the functions of reactor's geometry, operation principles, and the level of precursor mixing while determined by the delivery systems of the gas in flow designs. The TMG has been promoted due to optimal mixing of precursors as well as the compounding of reactor geometry of planetary radial flow reactor. Silvaco International 2001 found a new approach for uniformity control which was applied in a GaN radial-flow chemical vapor deposition system along with the planetary rotations of wafers. This technique provides complete physical insight for the process engineers so that they can utilize the knowledge to adjust the design parameter(s) to meliorate the uniformity. The results manifests that by the alteration of susceptor temperature, uniform films of GaN could be generated upon planetary rotations of the radial flow reactor systemMOCVD reactor possesses few parameters which required to be

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cautiously designing, and optimizing for effective operation. Among these parameters, nozzle (inlet) area, the distance between the nozzle and susceptor, and susceptor size are the most vital to prevent recirculation in the flow pattern.

(Chen.P.C, et al. 2006) explained that contributing to the attempts of reactor's design; the aim elaborations are required to be verified by real time growth runs. Those are defined by the reactor's load, potency, wafer size and period taken for a fully completed growth cycle. Optimization of the reactors' growth efficiency for the newly designed geometries is considered as time-consuming processes which should conceive the details connected to both the reactor's hardware as well as parameters of the processes. (Tanaka.T et al. 2001) stated that usually the design of the MOVPE is divided into two types with different designs of gas flow geometries, which are known as vertical type reactor and horizontal type reactor reportedly. Both the carrier gases as well as the precursor gases maintain their flow in the vertical direction for vertical type of reactors; whereas, in the horizontal type reactors, the gases flow in the horizontal direction. Aixtron 200/4RF-S MOVPE reactor, which is conceived for this dissertation purpose, possesses horizontal type of reactor's design. Figure 2.7 is showing the schematic of Aixtron MOVPE type reactor (Vesely.J.C, et al. 1974)

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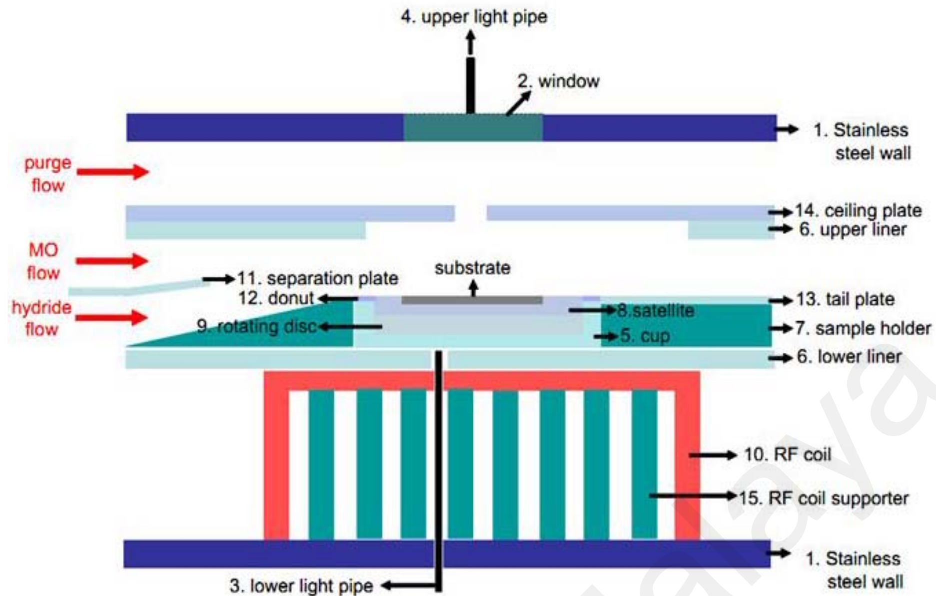

Figure 2.7 MOVPE horizontal type reactor
(AIXTRON,2007)

The importance of precise modelling of heat transfer from the CVD reactor's walls required to be emphasized. (Wakahara.A, et al. 1998) developed 3-D modelling of a horizontal reactor for Ga As deposition extensive analysis has been presented for the consequences of thermal diffusion and gravity on reactor performance. In that analysis, the bulk of the previous works have focused on the horizontal reactors designed for either Si or Ga As deposition (Nakamura. S). A few research works have been performed for modelling of vertical reactors and the growth of new materials which demands further investigation. Realizing the fluid flow and chemistry of the MOCVD reactor's processes and anticipating their performance. Nevertheless, it demands the ability to model the intricate chemical kinetics, fluid mechanics and transport phenomena in the process chamber. Due to these complexities, (Ahmet Erbil, et al. 2000) carried out an analysis on optimization work of recirculation cells in the reaction chamber, shape alterations of the reactors and therefore, conformal results were achieved through modification of cylindrical reactors in to the diamond shape reactors.

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Flow analyses in the experiment setup of cylindrical reactors were found to be vulnerable to the isolation from the adjacent wall of the reactors because of the abrupt expansion of the channel. But a gradual expansion of these ducts can optimize the separation of flow and thus smooth flow can be managed on the wafer surfaces.

2.3.3 Diamond Shape Reactor(Vertical)

Flow visualization describes that the recirculation cells are required to be eliminated from diamond shaped (small coned) reactor. Moreover, it is undesirable to design small cone since it results a very large distance of inlet susceptor. Because of such considerations, it has been found that gravity is proved as one of the significant parameters in varying the pattern of the inlet flow inside the reaction chamber where various geometrical parameters with considerations of the susceptor-inlet distance as well as the inlet tubes' diameter were found possessing the most crucial effect. Though excellent uniformity could be obtained through modification of these two parameters, no essential melioration was observed. Modification of the reactor shape and minimization of any recirculation cells in the reactor chamber can be achieved Acceptable results were achieved by changing the cylindrical reactor to a diamond shape(May, G. S., et al. 2000) as see in figure 2.8.

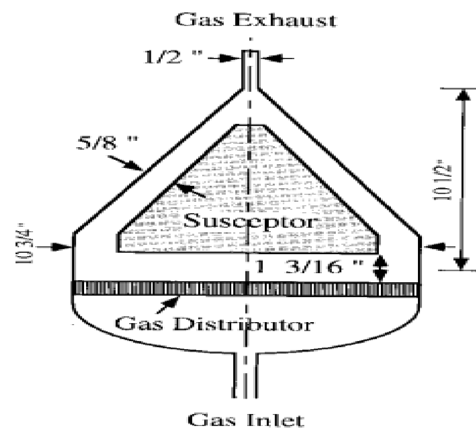

Figure 2.8Diamond shape reactor
(ZibaNami, Ahmet Erbil, and May, G. S., 2000)

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Thus, the design guidelines could be set to achieve an optimum MOCVD process reactor geometry on the basis of published documentations or research works, which should be coupled up to the practical considerations so that the geometries are realizable for smooth operation in normal conditions. In addition, (Winckenden.D.K, et al.1994) found out that rate of deposition and the uniformity of the growth rate are massively influenced by the angle between the direction of gravity and that of the GaCl inlet flow.

2.3.4 HVPE reactor Geometry

Process that involved in HVPE is the same principle process with MOCVD but the difference might be the geometry of chamber and type of gases involve. (C.E.C Ham et al. 2005) stated that the inlet angle of every tube in figure 2.9 play the important part in this research since it will influence the uniformity flow pattern of gases once enter the chamber. For thicker layers of this material hydride vapour phase epitaxy (HVPE) is a suitable technique and for small free-standing plate-like crystals, high pressure growth from nitrogen dissolved in liquid gallium is probably the only option. The domain for the computations represents the central 48 cm of the 101 cm long reactor tube.

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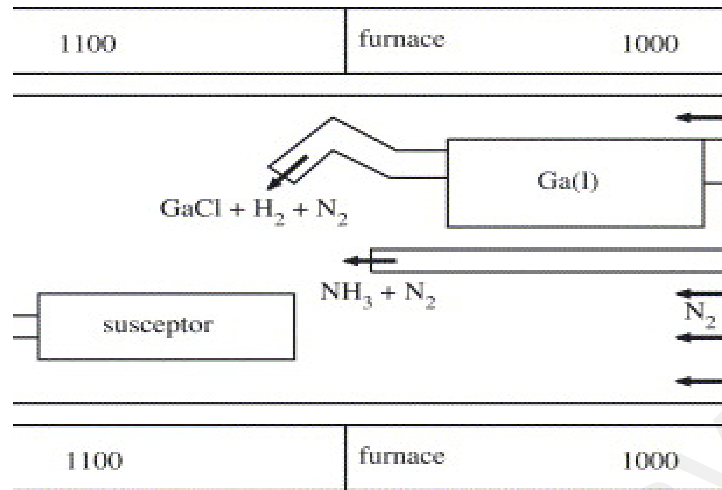

Figure 2.9 HVPE process of geometry reactor
(Winckenden.D.K 1994)

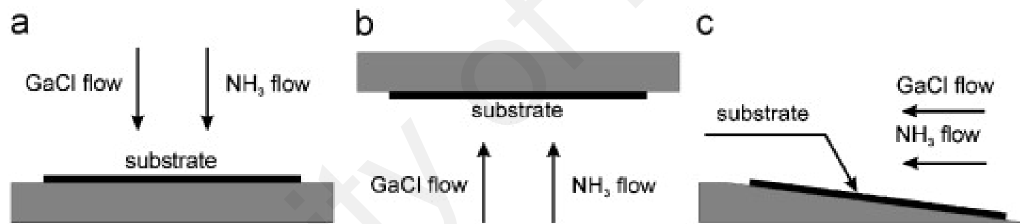

Figure 2.10 Types of flow direction in HVPE process
(Winckenden.D.K 1994)

Types of HVPE reactor recently applied in research industry and commercial production: vertical and horizontal as shown in figure.2.10 (a,b,c). (K.H Kim, et al. 20014). Attempts have been made to model reactors in order to study the relation between flows and growth (K. Naniwa, et al. 1990). There is a possibility of rotating the substrate to produced uniform concentration of reacting molecules (S.T. Kim, et al. 1998). Another alternative to improve the uniformity in horizontal reactors by using high gas flow rates at the expense of efficiency (ratio number of moles). While vertical reactors consist the two cases which is down flow and up flow reactors as seen in figures 2.10 a and b. The drawbacks on using down flow reactors is deposition of large

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particles dropped onto substrate surface will result as a parasitic growth on reaction chamber walls and structures. Another case is when up flow reactor is located under substrate holder as seen in figure 2.10 (b), this type of reactor potentially eliminates all disadvantages of down flow vertical HVPE reactors, but it is not well studied/optimised design. (A. Usui, et al. 1998) also revealed that the longer distance between substrate and gas flow inlets, it takes GaCl gas to reach the substrate. The initial pattern developed horizontal reactors with substrate positioned in parallel to gas flow figure 2.10(c). Besides that it will consume and wasted gas usage when reactor modelled with long of chamber.

2.4 Multi physics Simulation

The ANSYS Mechanical and Multi physics software which is a part CFD as well as the broad FEA tools. It incorporates pre-processing (such as geometry conceptualization and mesh development), solver, modules for the post-processing activities in a GUI (Faizul m.s et al.2009) as figure 2.11. CHEMKIN is both the developer and distributor for Reaction design modelling, which in the *de facto,* standardized to model the gas-phase as well as the surface chemistry so that the engineers can access in to the reliable benchmarks of the validation results leading to the saving of both expenditure and time for conducting research in every case study they perform for evolution. Reaction Design provides the multi-physics analysis tools for multiple flow in their software packages which facilitate the detail kinetics of such modelling for other engineering applications, viz. CFD programs, ANSYS and Solid Works Flow simulation 2011.

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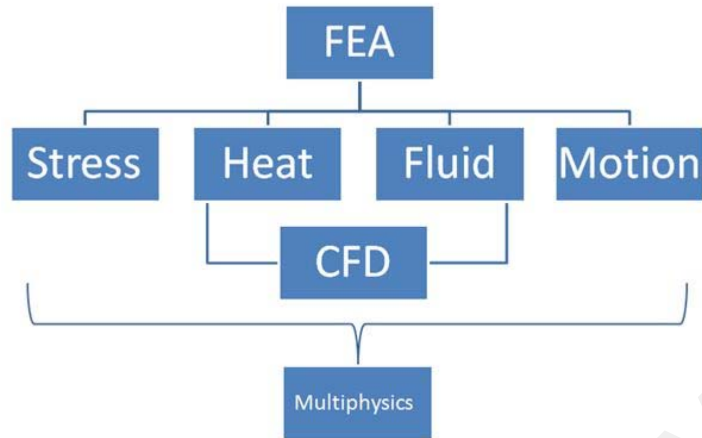

Figure 2.11 Graphical interfaces in FEA analysis

Multiphysics treat simulations the involvement of multiple physical models or individually simultaneous execution of multiple physical phenomena. As an example, the compounding of chemical kinetics as well as the fluid mechanics or combination of FEA with the molecular dynamics can be regarded as multi physics phenomena. Multi physics typically involve of the solution methodology forming the coupled systems for PDE equations described by the mathematical modelling. Coupled systems for these physics modelling in any simulation involves, such as the **E** and **B** (electric and magnetic fields respectively) for electromagnetism or pressure and velocity for sound or the real and the imaginary part of the quantum mechanical wave function. Mean field estimation is the other case to investigate atoms' electronic structure coupled with the electric field &the wave functions of electrons.

2.4.1 Semiconductor Simulation

Semiconductor process simulation is the multi physics modelling analysis to fabricate the semiconductor devices like transistors. This simulation type is a subdivision of electronic design automation processes and it was previously recognized as a sub-field of TCAD. The utmost goal of these process simulations is to accurately predict the

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doping dissemination, the stress dispersion as well as the geometry of the devices. Typically, the process simulation can be brought as inputs for the simulation modelling and that of the electrical characterization of the devices. Together with, the process and the device simulation lead to the formation of core tools to support the design phase's knowledge for TCAD or Technology Computer Aided Design. Conceiving the processes of integrated circuit design it is found that there is a successive combination of steps of decreasing level of abstractions where the logic synthesis might be in the extreme level and the TCAD might be regarded as the combination of phases where least quantity of abstraction is observed since it is nearest to the fabrication. Since there is an involvement of elaborated physical modelling the process simulation could be exclusively employed to assist in the evolution of single devices irrespective of their discreteness or partly of the integrated systems. Generally the process simulations deal with the modelling steps related to fabrication of semiconductor devices; like the transistors and concentrates to the steps of the front end manufacturing line. The distinctive inputs like temperature, pressure and chemical constitutions in the ambience etc. are regarded as the process conditions during the fabrication phases. The device simulation processes use the final outcome of the process simulations that is obtained as 2D or 3D structured devices.

2.4.2 MOCVD Simulation

CVD process features are found out through interactive influences of the hydrodynamic as well as the chemical kinetics which are regulated by the process conditions and the flow rates through geometries of the reactor. Till now, trial and error methodology has been adopted for the design optimization of CVD reactor's processes. In last decennary, the mathematical modelling that relate the process features of operation principles as well as the geometry of the reactor geometry have been formulated for various

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configuration of the reactors and that of CVD processes. These modelling features can be helpful enough for both the design of reactors and process optimization. Therefore, both the time and cost employed in the evolution of the prototypes and that of for the optimization of the process conditions could be reduced enormously. Thus a better reactor with an optimum process could be obtained in less expense. Moreover, mathematical models for the CVD processes might also furnish necessary needed perceptiveness into the existing physicochemical processes.

Design of the reaction chambers of MOCVD processes is largely established on empirical knowledge of their operation principle and flow phenomena. Generally, the expensiveness and time-consuming quality of such "trial and error" methodologies could make it inapplicable for efficient design and optimization of recent MOCVD processes (May, G. S., 2000). In this way, the flow visualization experimentations have provided significant knowledge into CVD processes flow phenomena as well as utilized to meliorate reactor geometries. Few simplifications could be constructed which largely cut down the complexities of computational effort required and the generated problems for the resolution of CVD processes' modelling equations.

2.4.3 Analysis Tool

The quality of the profile i strongly depend on maintaining thorough mesh density during simulation taking place. The mesh density should be as much as it meets the profiles' defects but due to the limitation of the computational resources to solve the diffusion equations for numerous mesh elements it should be controlled. Typically full CMOS process flow simulation might possess more than 50 types of mesh changing and it could be increased in a dramatic manner when adaptive meshing of those compounds is performed. There is a requirement of utilizing the interpolation technique to determine the values of the new meshes in after every mesh changing. But to avert the

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degradation in the interpolation technique's accuracy, it is essential to control the mesh changing and it could be easily obtained by keeping points when they are acquainted into the mesh. But this technique can cost a massive computational expenditure when the number of elements becomes quite large in amount. So a balance should be maintained among the interpolation errors, computational expenses as well as input parameters minimization so that minimal computational investment may provide acceptable and reliable computational analysis output, especially for 3D simulations. Generation of automatic adaptive meshing elements in the process simulation tools still faces limited success. Therefore, there is a necessity for the users to learn meshing techniques as well as the way to control the parameters which affect the mesh accuracy and thereby, the simulations results.

The most essential utilization of CAD tools could be regarded as to explore the new device technologies where many explorative simulations are conducted to provide the device designers a better knowledge of possible gains and disadvantages of an adapted technology. This can make the use of case demands for sequential simulations and analyses in between. To make it useful, lots of simulation cycles should be performed within the stipulated time given for explorative outputs and care should be taken to minimize the required simulation run time. At present, complete flow simulations for standard multi physics are frequently conducted with a combination of 1D and 2D simulations which just cost less than a few hours on a 2.6 GHz Pentium 4 type processing machines. To conduct these simulations for 3D modelling (from gate formation on), it may consume a minimum time of 24 hours if least accuracy is expected in the simulation. Therefore, the desired information from the CAD simulations should be derived from the simplified modelling treating as uniform depth(i.e. 2D simulation). But the 3D simulations have to be performed when there is a requirement of inclusion of device shapes along with the depth.

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2.5 CFD Analysis

At present, the world is certainly enjoying the renaissance of computational simulation technologies for which the rapid development of long time aspiring CFD modelling & analytical capacities have been increasing with less hardware expenses along with high capacity multi core system processing units so that the computational accuracy is claimable with less time consumption than it required a decade ago Regardless of the many substantial achievements, the advancement of CFD applications are meeting the raising demands from diversely emerging industries (figure 2.12)like biomedical, bioengineering, process industries, chemical engineering analyses, civil engineering applications, mechanical engineering applications in various fields like aeronautics, astronautics, nuclear and automotive industries and environmental engineering, etc.. Through utilization of the commercial software tool for CFD-CAE, induction heating, heat transfer due to radiation all these have been simulated collectively for an incompressible gas flow. The heating of the growth zone was numerically computed from the resistive joule losses for the RF-induced eddy current. Temperature as well as the flow velocities has been determined from the modelling through energy as well as the momentum equations as the profiles of gas concentration are found out from the conservation of mass and individual species. Since there is little variation of gas pressure in the system, it is considered as incompressible flow. Therefore, the gas density is considered as a function of temperature only. The thermal as well as the transport properties are estimated for the gases employing the kinetic theory of gases.

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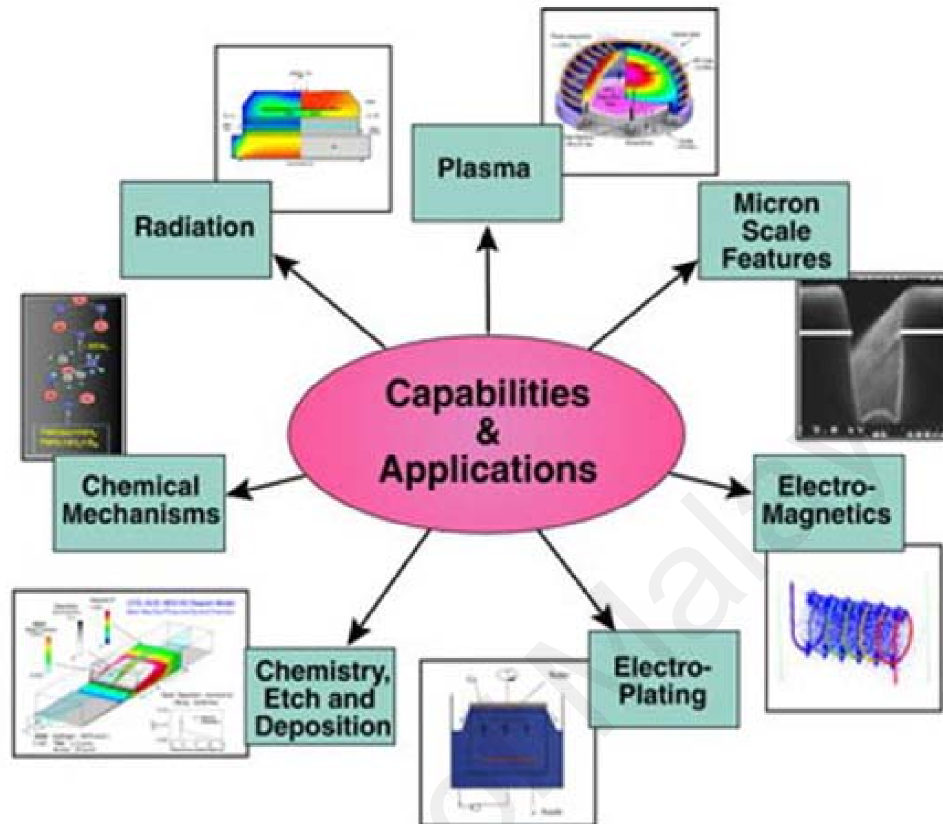

Figure 2.12 Application of MEMS in FEA analysis

2.5.1 Flow Pattern

The performance for optimization of the flow patterns inside the reactor as well as for growth parameters through simulation, which successfully generated layers of GaN growth free from the cracks. Bernardo et al has performed the simulation for the synthesis of GaCl as well as proposed that the rate of conversion of HC to GaCl should depend on the flow velocity of HCl. Self-consistent 3D computer simulation has been performed with flow dynamics analysis. Flow patterns mostly involved among the geometries of the reactor chambers, tubes and pipes etc. or to be determined and analyzed from the patterns of multi-physics encompassing the chamber on the basis of shape as well as the geometry itself. Relationship between flow pattern and other

parameters is more important to investigate for comparison between the experimental as well as the simulation results. At the same instant, surfaces by emended flow patterns along with the mixing point of group III and IV compounds minimize the contact between gases and parasitic deposits prior the growth reaction (A.S Segal, et al. 2003). Hence, the observation from direct flow pattern has been utilized successfully to alter the reactor's hardware and stabilize the growth conditions (Dyakowski, et al. 1993).

2.5.2 Temperature Consideration

In the flow simulation method, the involvement of flow with the temperature parameter plays an important role to sustain and maintain the conditions of certain application, especially, in the semiconductor industries. It is widely known that semiconductor application is very familiar with thermal heat conduction that might affect the growth surface. The insufficiency of temperature utilization will affect the uniformness of GaN wafer and the geometry of the reactor instead. Temperature inside the reactor is influenced with chemically responsive surfaces of GaN crystal. These chemically responsive surfaces of the reactor's side walls are formed with the boat in liquid terms. A quasi-thermodynamic model is utilized to depict mass exchange within the vapor as well as solid surface.

2.5.3 Velocity distribution

The corresponding linear velocities changes from 70m/s to 105m/s. Depending on volumetric flow, comparatively higher inlet velocity can be experienced where the mean flow rate of gas inside the reaction chamber might be substantially altered later if required. The maximum velocity is observed at the nozzle inlets. Temperature and the pressure are set as constant thermodynamic parameters and the used constitution of hydrogen and that of nitrogen are utilized in 1:2 ratios with the flow parameters of thermodynamic pressure and temperature set constantly. The flow of the gas is

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considered as incompressible as the pressure varies very little and therefore, the density of the gas is considered as a function of temperature.

2.6 Application of MOHVPE in Semiconductor Industry

Researchers are focusing on the issues of improving the design geometry of the reactors and optimize the flow pattern uniformity in to 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 in to forward. The HVPE method, defined as the potential growth technique so that both the large size as well as the thick cystal layers of GaN can be furnished (Zhao Bao, et al. 2005) his 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 NH3 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 metal organic halide vapour phase epitaxy (MOHVPE) has been proposed. These are the results of hybridization between the growth reactor for MOVPE and HVPE simultaneously.

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CHAPTER 3 RESEARCH METHODOLOGY

DESIGN CONSIDERATION FOR THE REACTOR GEOMETRY

3.1 Modelling growth chamber

Based on the findings from the literature review, the design considerations of the growth chamber can be divided into a few stages. Before describing those stages, it is to be mentioned that the initial point is to define the assessment method, which method would be considered as suitable design for the growth chamber of MOHVPE process based on the requirements or purposes. Therefore, the first stage, design for geometry of the growth chamber should be presented. The second stage is to conduct the simulation analyses on geometry of reactor design by following the assessment method. They will come out with result analysis for verification of simulation data need to define. The third stage is to optimize the geometry of the conceived model and obtain the final simulation result having a better performance, i.e. growth uniformity. The parameters that will be considered are the flow pattern, temperature distribution and velocity to improve in terms of performance of growth chamber itself since this is new approach of evolution in semiconductor industry.

Conducting the modelling and simulation for evolution of MOHVPE process technology has becoming more and more intensive over last few years progressively. Recently, modelling may be used for both processes and reactor optimization purposes. Based on new model of MOHVPE, previous design criteria from MOVPE and HVPE growth reactor specifications are identified. The advantage of such system is the possibility to simultaneously grow thick (high growth rate) and thin (low growth rate) GaN-based layer on a target substrate, without exchanging growth instruments

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when both thick and thin layers are required on the same substrate. Therefore, it reduces surface contamination, layer stress and substrate bowing during cool-down and heat-up process, resulting samples with a lower threading dislocation density and higher film quality.

3.2 Schematic Diagram of MOHVPE

The proposed schematic diagram of the growth chamber in metal organic halide vapor phase epitaxy (MOHVPE) reactor is presented in figure 3.1. Based on the previous designs of MOVPE and HVPE reactors' specifications are identified for the new modeling of MOHVPE reactor having horizontal duct. This modeling 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 40cm length horizontal direction with one outlet tube where the gasses dispenser.

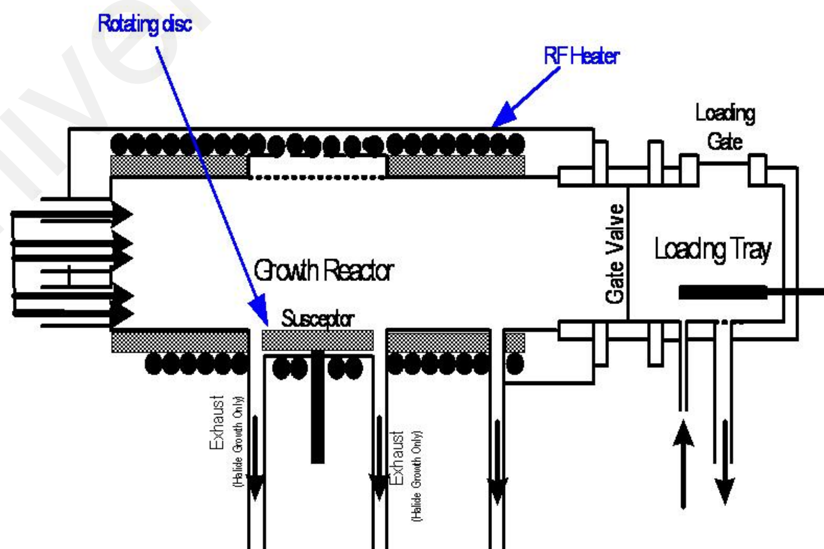

Figure 3.1Schematic Diagram of MOHVPE Growth Chamber

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3.3 Description of Methodology

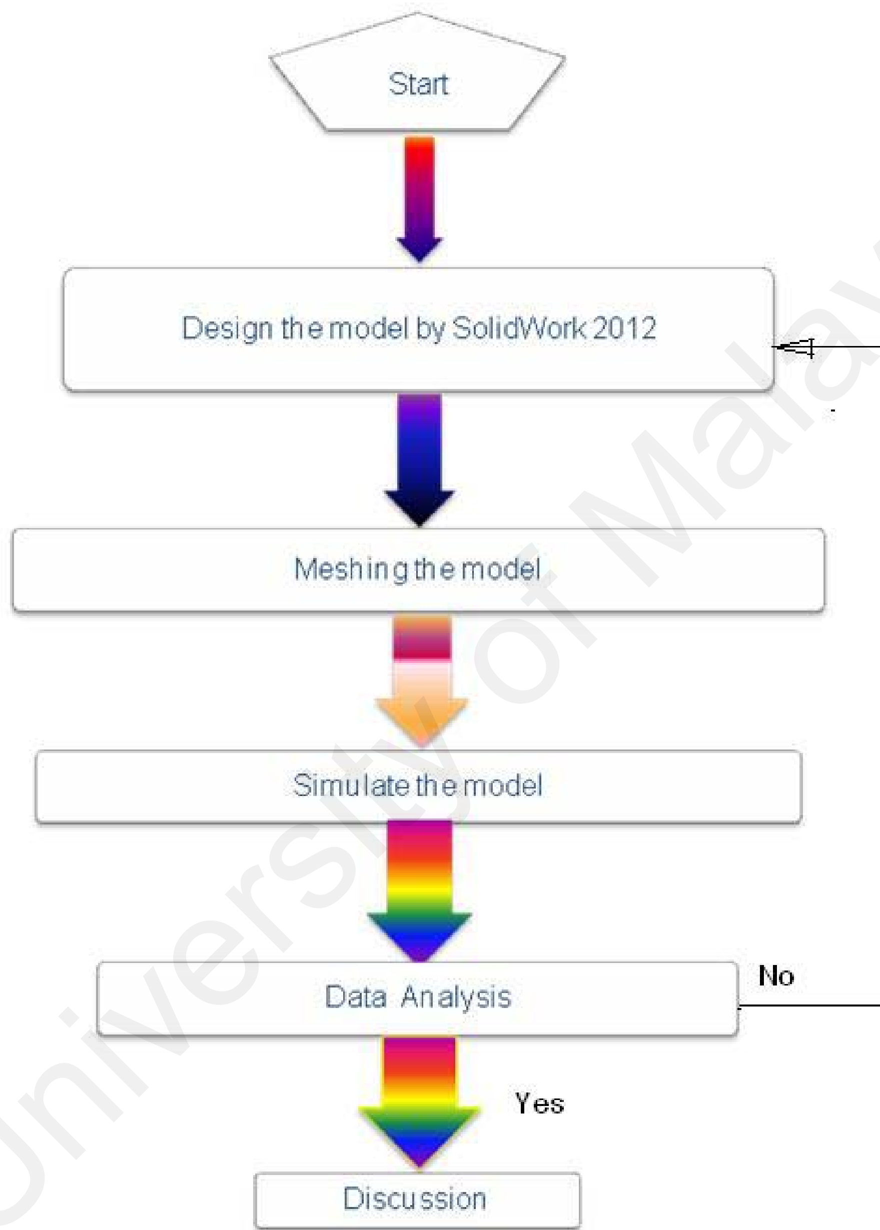

Figure 3.2 Flowchart for methodology stage

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3.3 Detail Design of MOHVPE Reactor

The detail design criteria for the MOHVPE processes have been chosen on the basic of their applications. For the conceived model, the growth chamber specification is shown as in figure 3.3.

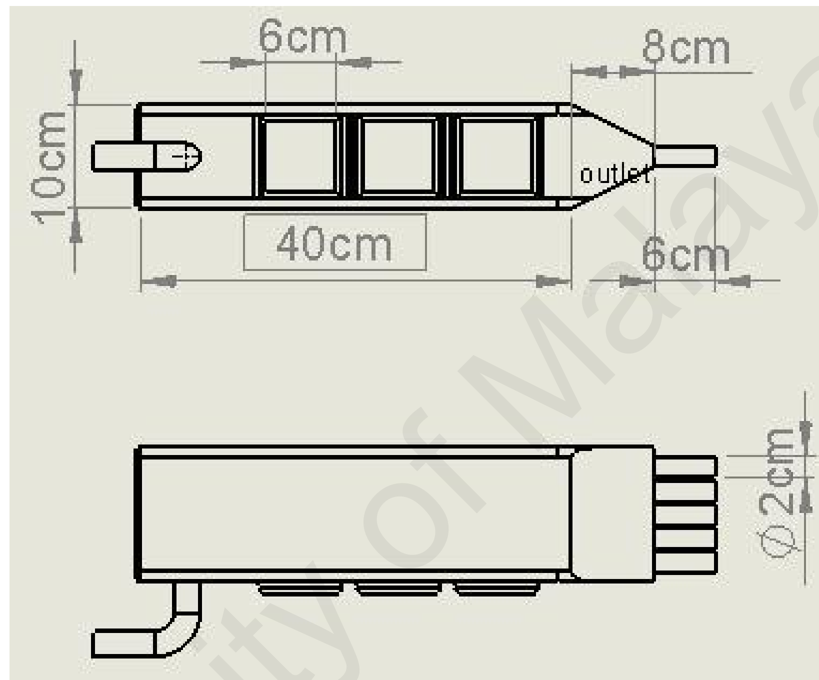

Figure 3.3 Detail dimension of chamber

Modelling of this reactor was performed on 2D and 3D model designed by the Computer Aided software tool SOLIDWORKS (Version 2011). This is a horizontal reactor in order to reduce the computational time.

The computational analysis runs up to 10 h on a 2.8 GHz Pentium i7 processor and 4.0 GB RAM. The following explanations are assumed with final design has come out in very detail information:

i) The long reactor is estimated to be 54 cm including nozzle inlet. To eliminate gases consumption to be waste with no function of it.

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ii) In every single nozzle inlet, gas will flow in every different inlet based on MOHVPE process gas. This reactor is constructed from quartz wall components.

iii) The major part in this research will not be considering the mixing of gases and growth process, but will be focus on the reactor design with flow pattern inside the chamber as this is a new development technology.

3.4 Process Flow in Analysis Modelling

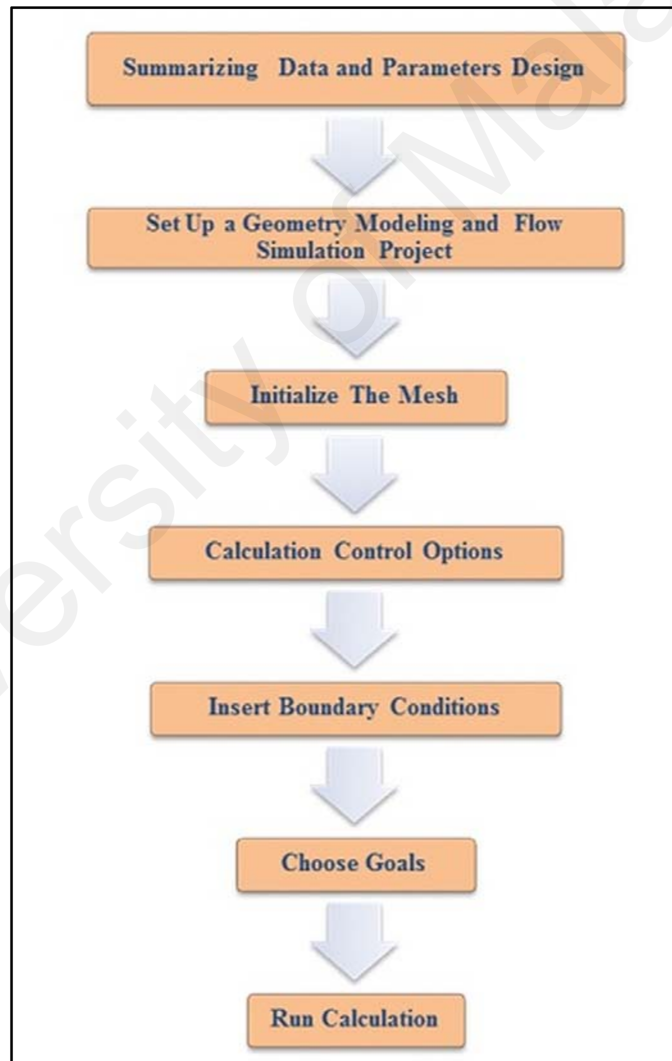

Figure 3.4 Flowchart for fluid flow analysis using SolidWorks Flow Simulation

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3.5 Previous Design Consideration in new development MOHVPE

Semiconductor system in HVPE produced molten gallium and HCl gas use as a precursor. It is nearly equilibrium due to high growth rate (thick film) temperature. Molten liquid gallium that kept in the boat located at the bottom of reaction chamber in front of the inlet, as shown in figure 3.5. MOHVPE GaN and its alloy are grown by reaction of metal organic precursor with NH_3 in precisely controlled an ambient temperature and pressure. It is produce non-equilibrium process in lower growth rate which is suitable for growth of device grade thin film. Combination for this process will develop growth instrument MOHVPE in single reactor. The nitrogen and remaining gas are transported through the pipe to the outlets depends on the technical solutions adopted in the particular reactors. The outlet design MOHVPE was similar with outlet design for HVPE. The outlets do not affect the gas flow even for a relatively short pipe used for the transport of the reactions to the outlet.

MOCVD can be held with single zone temperature to growth the TMG and GaN in one phase process. While MOHVPE is held with two zone area with different temperatures. In terms of growth rate, MOCVD provide high growth rate while MOHVPE produce low growth rate. MOHVPE is choose for horizontal direction because good uniformity for gas flow to spread out due to that it produce low growth rate compared to vertical direction, produced uniformity for substrate cause the gas flow is focus on certain area directly below the inlet an it will produce high growth rate.

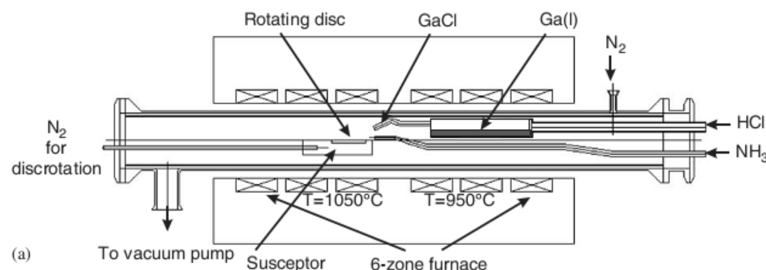

Figure 3.5 HVPE reactor design (P. Kempisty,2006)

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3.6 Modelling Analysis

Computer aided design tool SolidWork 2011 codes can be divided into nine modules, which is as shown in the schemetic figure 3.5. It contains several interacting software for instance stands for Complete Aided Environment and is a pre-processor. CAE is a graphical environment where models can be created or imported from other CAD-systems. Multiphysics simulation SolidWork 2011 is a post-processing tool that visualizes the result of an analysis. This chapter describes the modelling procedure for a portable hard disk that is exposed to a free fall.

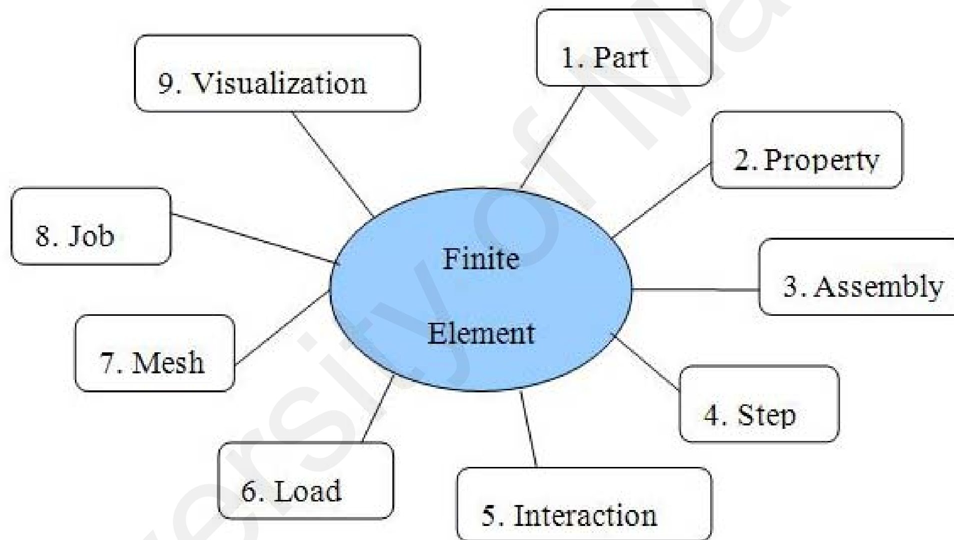

Figure 3.6 The scheme of nine modules that facilitate the use of pre-processor

There are three phases in FEA:

1. Pre-processing: To develop a finite element mesh to conduct the mathematical analysis. Properties of the materials as well as the boundary conditions are also defined in this phase.
2. Solution: Governing equations are derived as matrices based on the modelling and they are solved as per the user input values in the post process phase.

3. Post-processing: The results obtained from solution are checked for validation and acceptance against the available experimental values (i.e. displacements as well as stresses).

3.7 Pre-Processing Model Geometry

The enclosure body is a three dimensional solid structure. Hence, a part of three dimensional deformable with extruded solid base feature was created and the figure 3. 6 below is the 3D wireframe of the model located three substrates holders inside. The 2D cross section area is defined in figure 3.7.

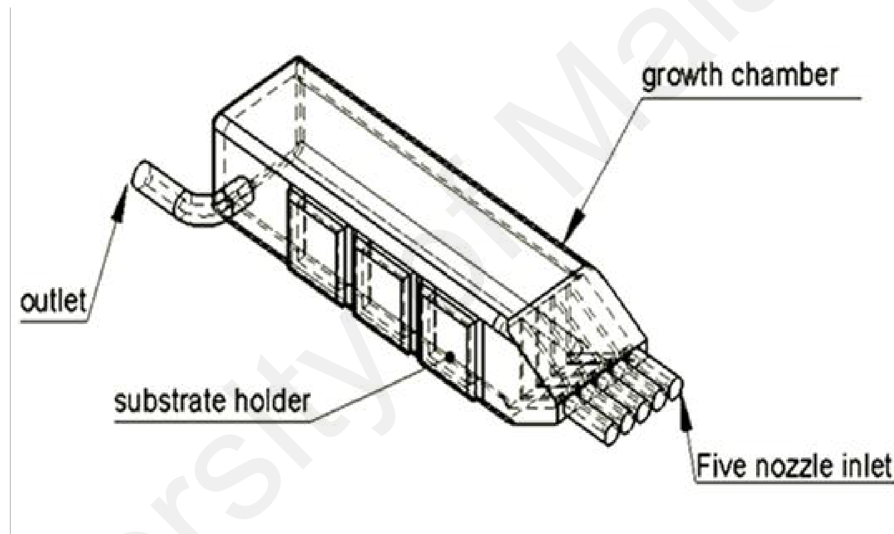

Figure 3.5:Modelling view

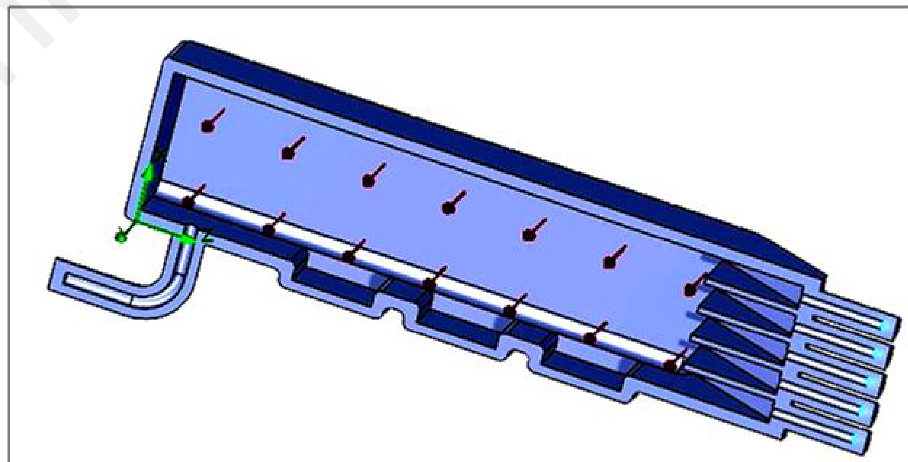

Figure 3.6: 2D cross section view

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3.8 Nozzle Inlet Modelling

The main parameter 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 (ρv2) of the entering fluid or air. In every 5 single nozzle inlets inside the reactor, figure 3.8 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 area (Kempisty. P, et al 2006). The area after small inlet it expand with wide area to ensure gas flow after the barrier obtain uniformity of entire chamber.

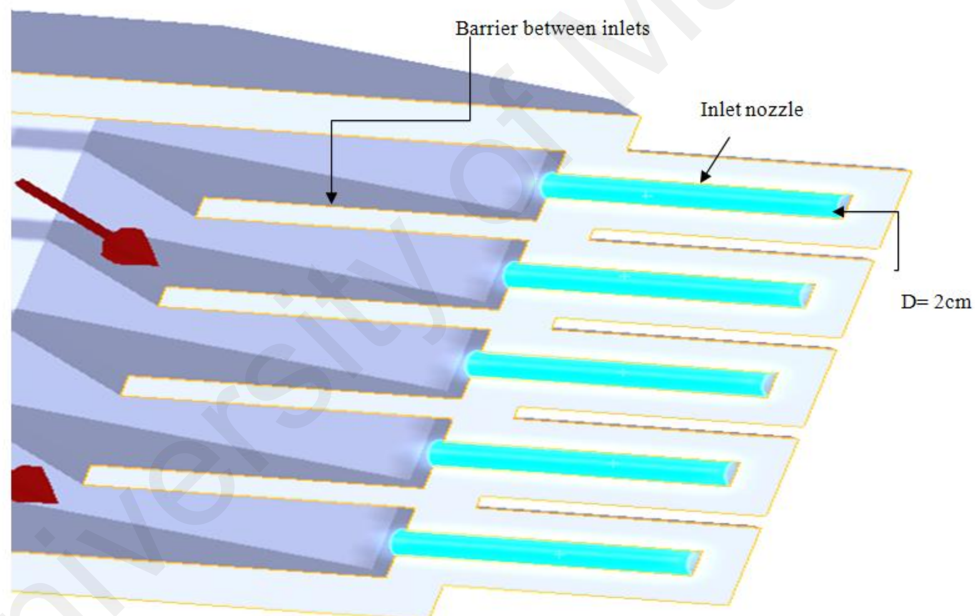

Figure 3.7 : Inlet nozzles as the main entrance

3.9 Finite Element Analysis (Mesh Generation)

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

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ensure the precision of the solver to obtain acceptable results. For an accurate result, a triangular mesh with a minimum element size 150nm was used. Geometry of the chamber was solved using finite-element SolidWorks code 2011. Figure 3.9 (a,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.

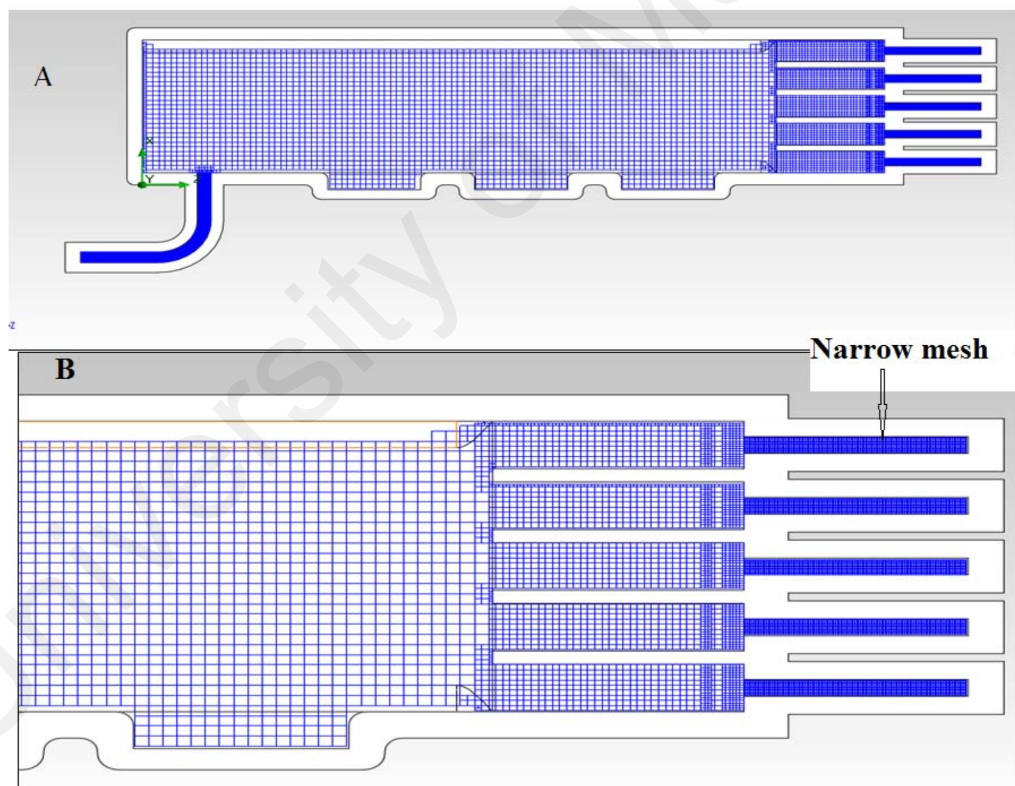

Figure 3.8 Meshing generation geometry of Reactor chamber (A) Full body meshing (B) close up narrow inlet

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The SolidWorks Flow Simulation's mesh comprises of rectangular parallel piped cell elements. The essential information about mesh generation is that the smaller the element size of a region in the model the more the solver solves the model precisely in that region. In this simulation, it should be kept on considerations that the finer mesh elements of fluid flow regions should consume more solution time and massive RAM space, therefore the solution must take significantly long period of time to achieve the convergences in a standard work station. The meshes in computational tools are generated through utilization of automatic mesh generation setting but they require the user input for minimum gap setting, element size setting and the minimum thickness of the model's walls for appropriate quantifications.

3.10 Material Selection

Quartz is chosen because of the strength and durability to withstand the heat without cracking. The added resin makes them often more durable than natural stone which is also a prominent advantage an addition to the above qualities of quartz, their countertops are almost free from maintenance works, they are wholly non-porous (i.e. they don't take up strains or spills) due to their generation from delicate quartz crystals. The conceived quartz material's parametric properties are given in the table 3.1.

Table 3.1properties of Quartz

Material properties of the quartz	**Value**
Density (g cm^{-3})	2.2
Compressive strength (MPa)	1100
Coefficient of thermal expansion ($x10^{-6}$ K^{-1})	0.54 @ 20-1000°C
Melting point (°C)	1715
Specific heat (J K^{-1} kg^{-1})	670-740 @ 25°C
Thermal conductivity (W m^{-1} K^{-1})	1.46 @ 20°C
Upper continuous use temperature (°C)	1100-1400

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The technical solutions govern the design of the conceived reactor's outlets (figure 3.10). The particulars of the reactor outlets are regarded as vulnerable technical issues by many manufacturers therefore, these discussions are not mentioned in this section for commercial ethics. It is assumed that the flow of gas is laminar within the continua and it is Newtonian fluid. Due to axis-symmetry, the modelling simulation can be performed treating a 2D axis-symmetric geometrical model. For horizontal reactors, approximate boundary layer has been considered with the walls though they are well insulated to assure adiabatic thermodynamic situations for walls as per the quasi-thermodynamic surface chemistry models. In the cases of MOHVPE processes, as it is even in rudimentary conditions the real time parametric values those influence the processes were not considered for all inlets as well as for all gases used.

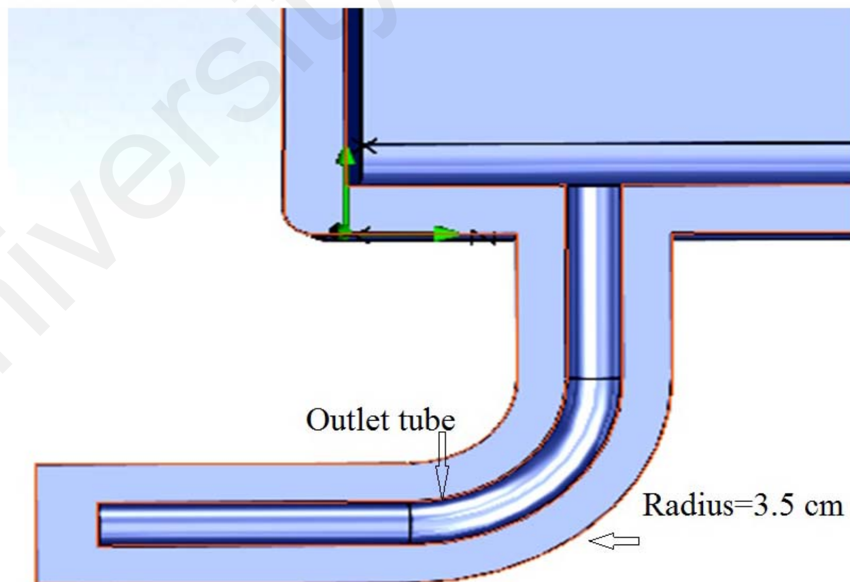

Figure 3.9: Design of Outlet

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3.11 Simulation of Flow Pattern MOHVPE Growth Chamber

Firstly, for high quality flow simulations, different types of gas flow rates, velocities and temperatures are considered in all of the 5 inlets individually in every substrate holders. The consequence of slow rotations of the substrates on the gas flow is disregarded in the two-dimensional transport modelling by the Computational simulations of reactor's geometrical model. This was conducted using the CFD-Solidworks flow simulation. The objectives of this simulation are to predict the performance of this design idea for the conceptualized flow pattern. Therefore the assessment method needs to be specified as the issue involves performance observance stage by stage. For the initial steps, as mentioned earlier, the three holder substrates will be considered. Then the optimum place for the holder substrates will be determined. It should be noted that, since this modelling is very recent, novelty approach have been discussed before and their significances are presented on the following observations, therefore many assumptions need to be considered due to rudimentary analyses stages.

3.11.1 Calculation Control Options

Figure 3.11 manifests the computational control options of the simulation through which the dependent parameters are influenced in the simulation and on the time required for completion of simulation as per the setting presented here. From the table, the maximum time of calculation was set as 36000 seconds and the intention was to contract the time spent for simulations.

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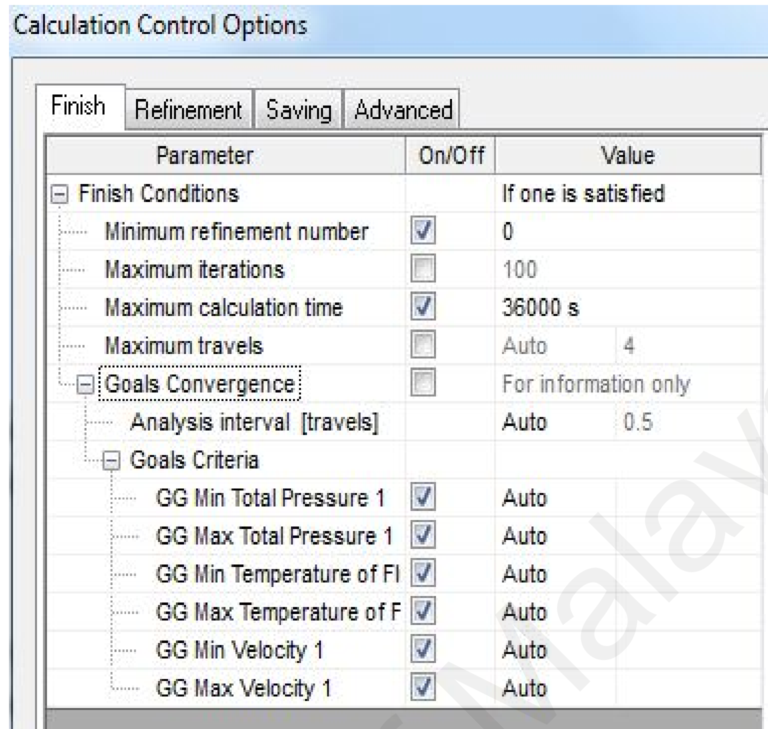

Figure 3.10 The setting for the calculation control options

3.12 Boundary Condition and Parameters Consideration

Before setting up the model, all the walls of the reactor's inside are set as no-slip and thermodynamically adiabatic for wall boundary conditions except for susceptor and furnace walls which have the temperature as set in the parameters of simulation. While the initial boundary conditions for the gases can be listed as follows:

(1) Gas flow is presumed to be both laminar as well as turbulent;

(2) Gas substance is Newtonian and in the continuum region;

(3) The transport species are considered as self-consistent in the 3D computational simulations.

The transport species consider the hot walls as insulated, flow is dynamic, temperature is well distributed and the velocity of the gases is defined. And the surface chemistry is consistent for the used parameters in the boundary conditions. The inner diameter of the quartz reactor is 35mm in substrate zone. Based on the type of the analyses for the problems defined model chooses whether this will be regarded as an internal type or external type. In this case, internal analysis type was chosen. Apart from that, gravity also influences the simulation as per the setting of parameters in the pre-processing phase.

The influences of the parametric quantities like the ratio of nitrogen and hydrogen in carrier gas, the pressure inside the reactor (maintained between 10000KPa as well as 101245 kPa and temperature of the growth chamber have been studied. Once inside the reactor, the substrate zones were heated to the growth temperature under $N_{2,}$ H_2 and NH_3 fluid flows. Figure 3.12 stated out the parameters setting before running the simulation.

Parameter	Value
Parameter Definition	User Defined
⊟ **Thermodynamic Parameters**	
Parameters:	Pressure, temperature
Pressure	101245 Pa
Temperature	1135 K
⊟ **Velocity Parameters**	
Parameter:	Velocity
Velocity in X direction	80 m/s
Velocity in Y direction	0 m/s
Velocity in Z direction	30 m/s
⊟ **Turbulence Parameters**	
Parameters:	Turbulence intensity and length
Turbulence intensity	2 %
Turbulence length	0.00100005 m
⊞ **Concentration**	

Figure 3.11Parameter setting inside reactor

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Goals of the problem stated are the pre conditions employed to cease the iteration of the analytical process. They also check the further miscalculations of the targeted parameters and foreshorten the full solution processing time of the considered solver. There are numerous types of goals to be implicated from this conceived simulation; in this case, the flow field is observed through the global parametritic quantifications. The inlet flow velocity is set as a constant quantity of 0.05 m/s for all categories of simulations at each inlets (figure 3.13). But the temperature is varied between 1273.2 K and 1473.2 K in all the simulations. In the meantime, the pressure is set as 0.1 MPa for the opening of the pressure.

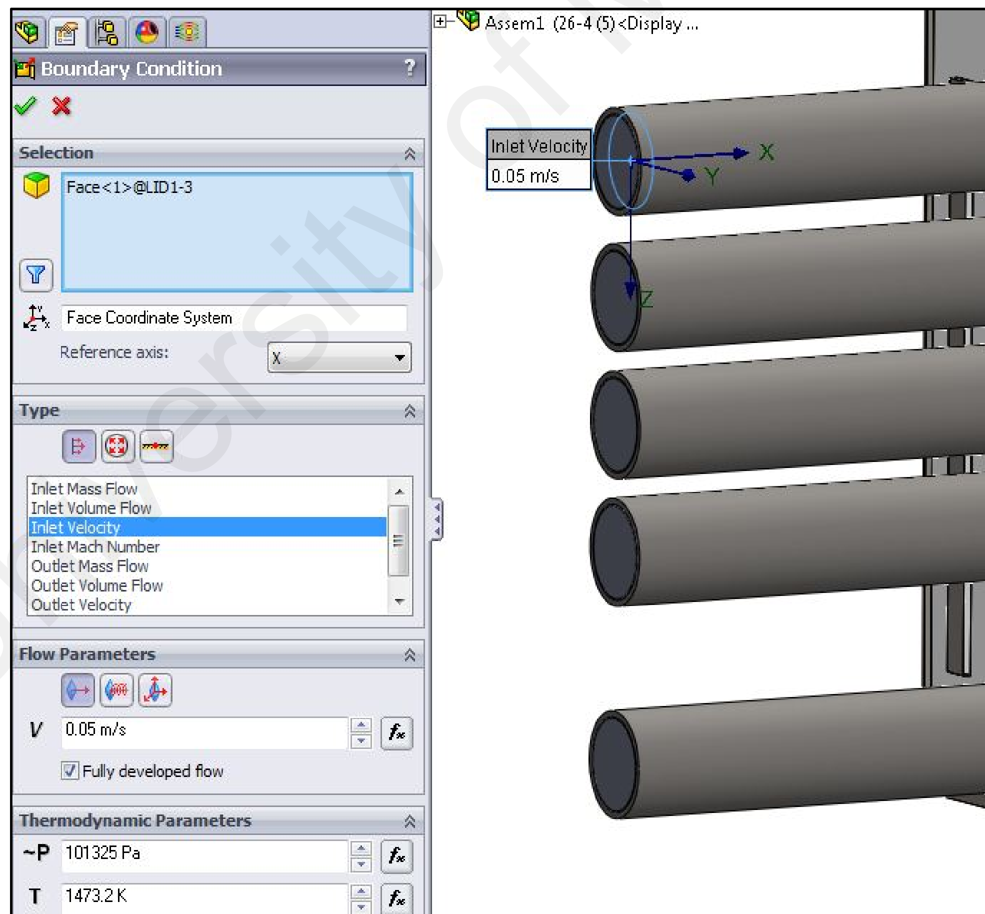

Figure 3.12 The setting boundary condition at inlet nozzle

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3.12.1 Temperature Distribution

With the objective of having more global parameters and applicable to several different designs of apparatus, detail design is correlated with the values of dimensionless numbers calculated. Because of the instability of GaCl at temperature below 600^0C, the chamber of the reactors must be maintained above that level of temperature. Maintaining the heating system at every level is also necessitates due to risk of deposition of parasitic chlorides of ammonia. The chamber is divided in to two zones with different temperature. The inlets are extended towards the substrates as well as the temperature of the wall was set from 550 ^{0}C; the 5 inlet nozzles are set for flow under the room temperature of 27^0C for each inlet. While after pass the barrier the temperature in heat up between 1200^0C -1000^0C .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. NH3 also flows through inlet 4 and 5 ranking from the bottom chamber. Hydrogen is heated up to 800 ^{o}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. Central holder is stressed out to make clear of the best position for the required activities as observed in figure 3.15. 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.

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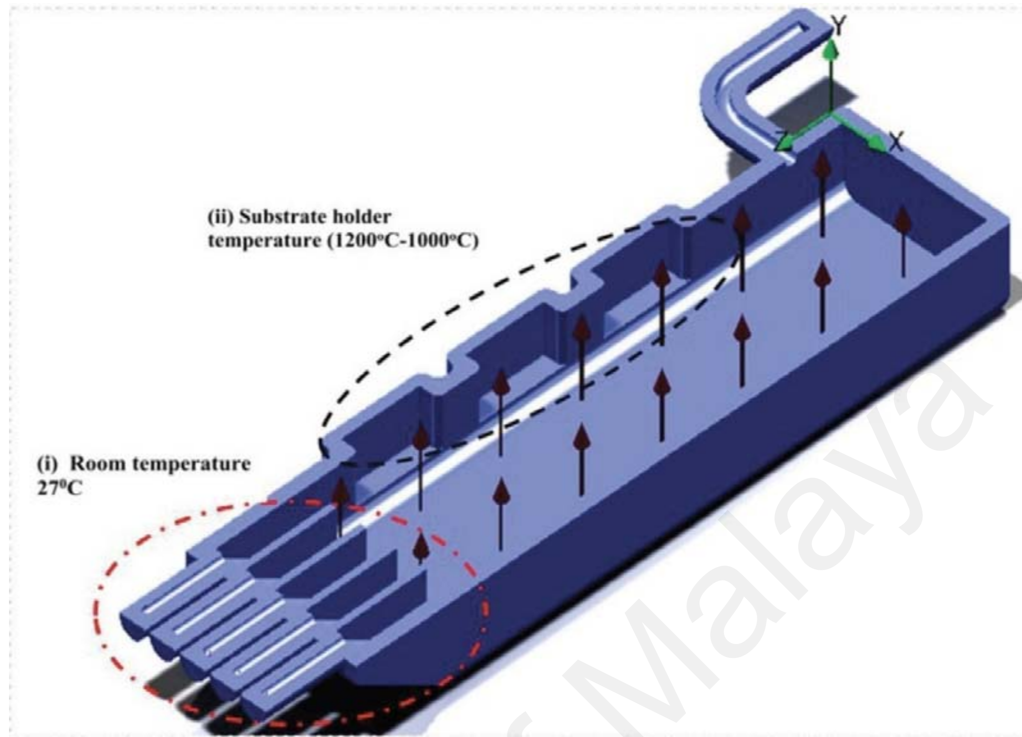

Figure 3.13 Two zone area of temperature involved. (I) Inlet nozzle area (II) substrate holder area

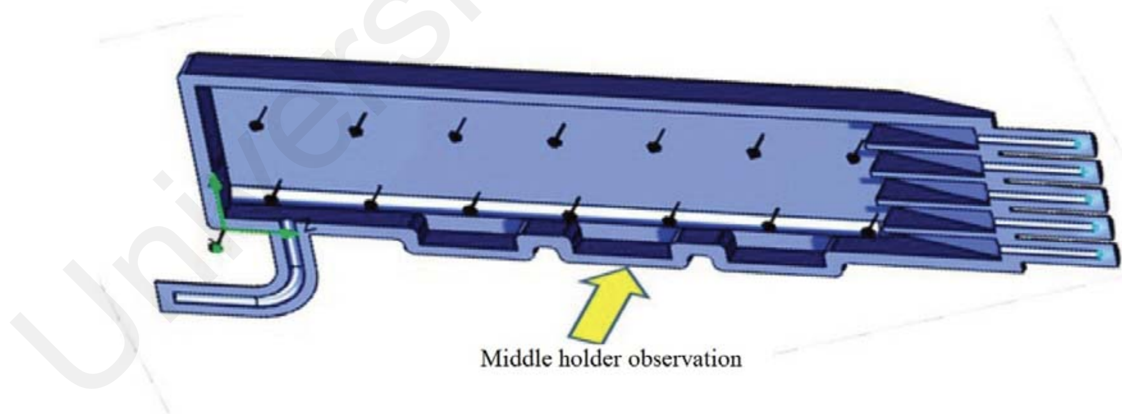

Figure 3.14 : Middle holder is observed in simulation run

3.12.2 Velocity distribution

The inlet velocity of the gas in flow in to the chamber was maintained as 0.5m/s in every cases of simulations. Depending on the volumetric flow conditions of

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the gases, the inlet velocity might be regarded as relatively higher but they can be modified in the reaction chamber as per necessity at later times. The nozzle inlet velocities are found as maximum velocities on the basis of observations. The composition of hydrogen and nitrogen are used in 1:2 ratios with the flow parameters of thermodynamic pressure and temperature set constantly. While for ammonia is used 1:1 with nitrogen. The gases are considered as incompressible as the pressure fluctuations are not significant. Thus the gas density is considered as temperature dependent only.

3.12.3 Pressure and Flow Pattern Distribution

Unless it is mentioned, pressure is one of the thermodynamic parameters in all simulations conducted here. In the horizontal flow type reactor used in this case the gases were fed through the inlets located on the horizontally right side of the reactor chamber. In this analysis, the energy as well as the momentum equations provides the gas flow velocities at any positions while their concentration profiles could be obtained from the conservation of mass. As in the distinctive implementations, the constitution of the mixing is prevailed by the molecular nitrogen (N_2) (usually about 90%), the viscosity of the nitrogen could be considered as that of the mixing gas constituents all together for the application of Navier-stokes equation. The total amount of pressure inside the system for this simulation is considered as 0.75MPa, which is usually utilized in the conceived system of analyses tool. The pressure ranges from 0.8atm-1.0 atm with addition to a NH_3 concentration ranging from 0.3% to 1.2%.

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CHAPTER 4 RESULT &DISCUSSION

4.0 Introduction

Result and analysis data are taken from the simulations conducted for analysing the problems stated while the objectives were mentioned for this dissertation. By using an appropriate computer simulations program, can be effective and less expensive tool to analyse the design alternatives and to carry out the best optimization holder by investigating how the flows' patterns are featured based on the reactor geometry. The use of suitable computational models for assisting in the development of prototypes or to improve a particular design can also reduce the amount of costly physical testings for iterative/ trial and error stages.

4.1 Analysis Modelling

The simulation results can be utilized to determine 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 24cm (1), 34cm (2) and 44cm (3) from the inlet nozzle to substrate holder is seen in figure 4.1 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 3 times with both MOVPE and HVPE ;/before the

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gases start to enter. This is to make sure that the whole chamber is completely clean and free from dust and other pollutants.

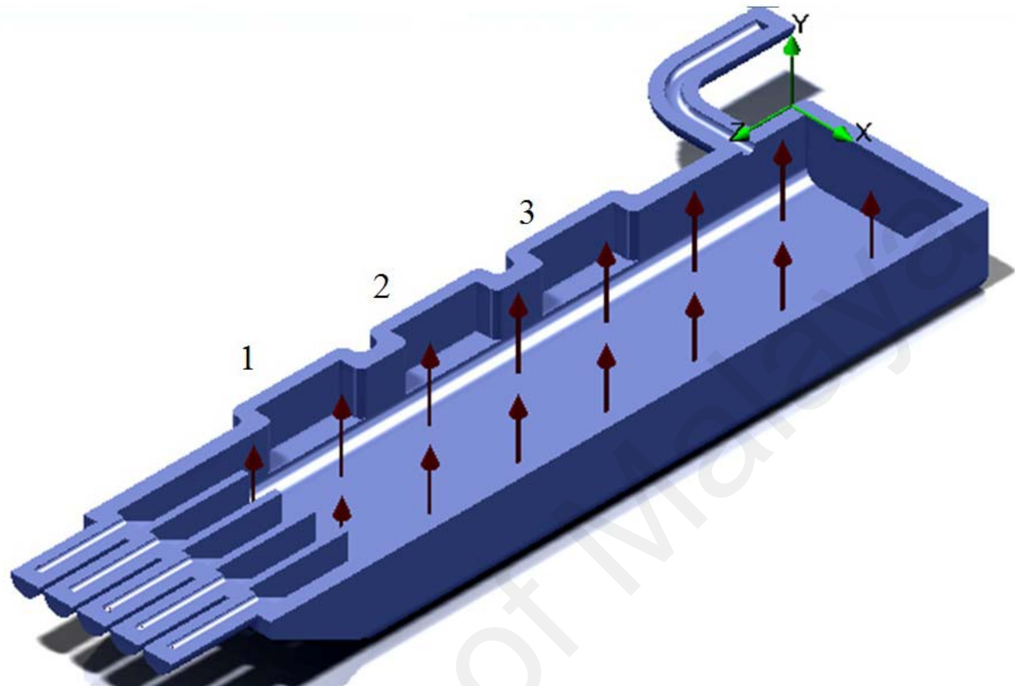

Figure 4.1 2D cross section view with 3 substrate holder allocated

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.

4.2 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

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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 figure 4.2.

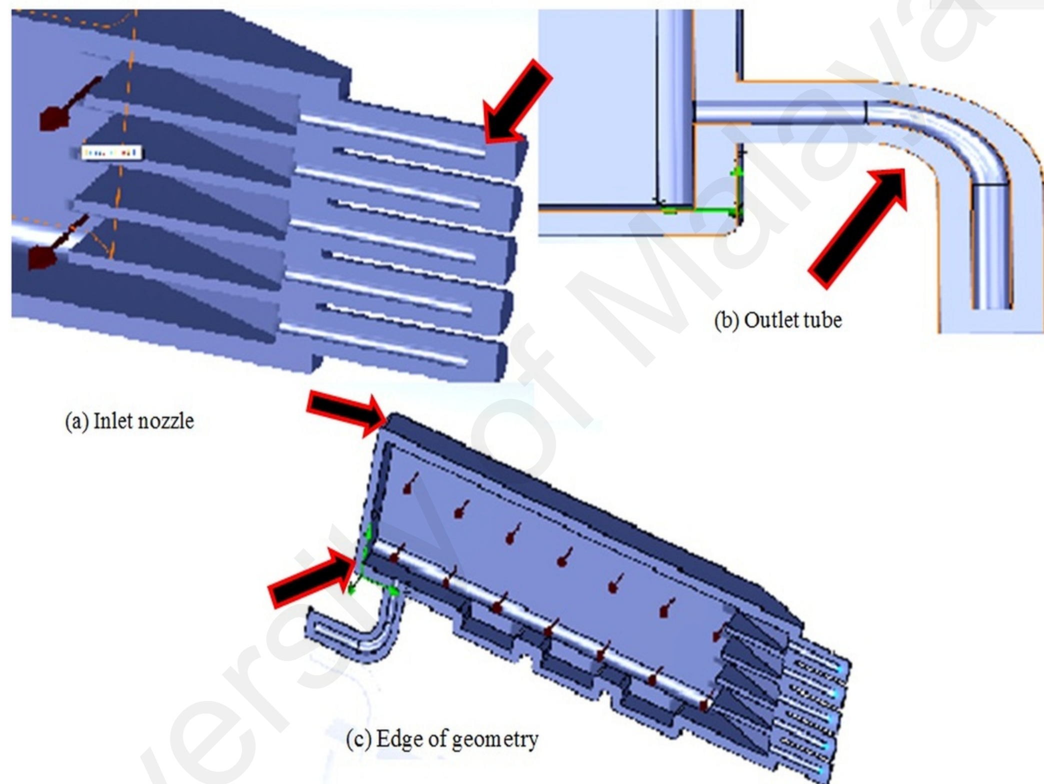

Figure 4.2 Part of the critical that possibly affect the geometry

4.3 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,

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the observation on temperature rate is analysed from 1200°C to 1000°C and it explained the three situations of temperature.

4.3.1 Simulation Result at 1473K

The colour contour is used to demonstrate the distribution of temperature as obtained from the simulations for reaction chamber phenomena at user defined boundary conditions. From the captured figures, obviously when the flow patterns are observed right after the system starts and in various conditions can be defined from the contour colours, like blue being the starting value of a process or lowest value of any parametric quantification, whereas, the red colour is the maximum distribution of any parametric analysis. In the case of temperature distribution as per simulation conditions at 1473K, the gas is distributed more evenly through all the process in whole chamber (figure 4.3).

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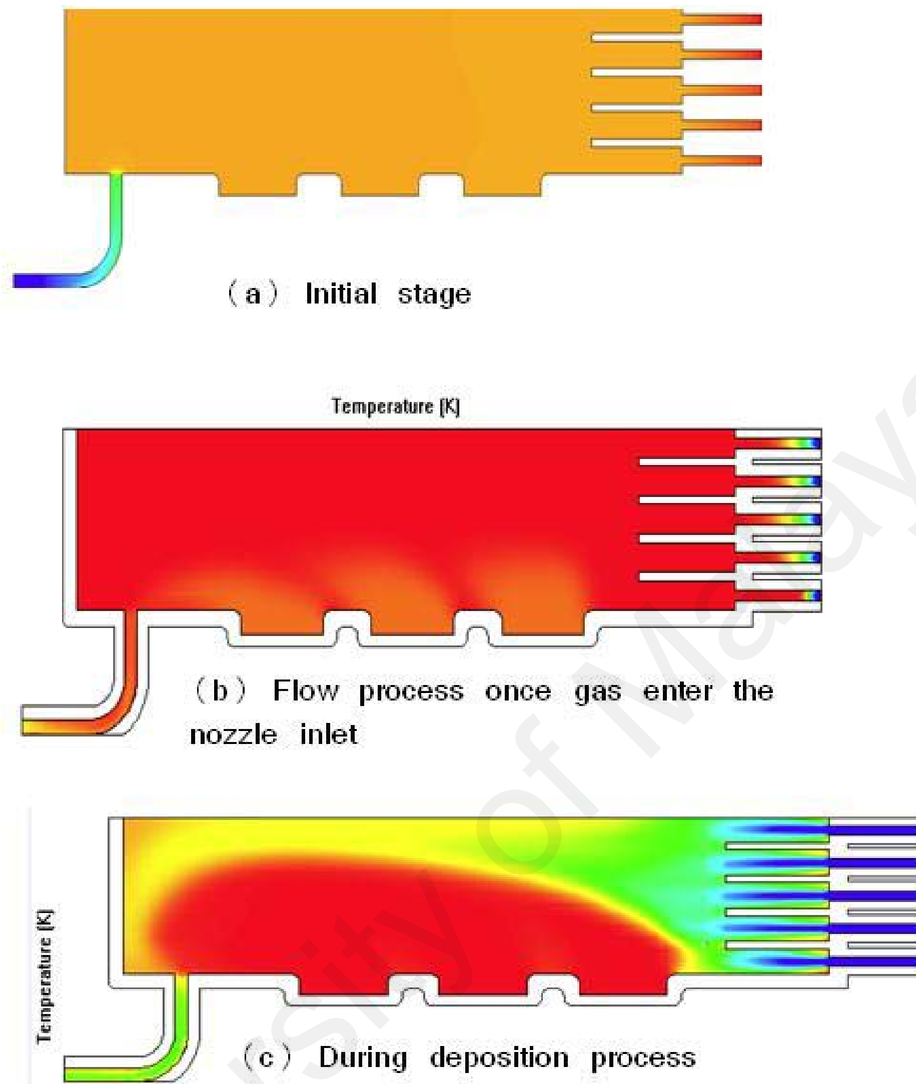

Figure 4.3 Captured figures 1473K temperature distribution

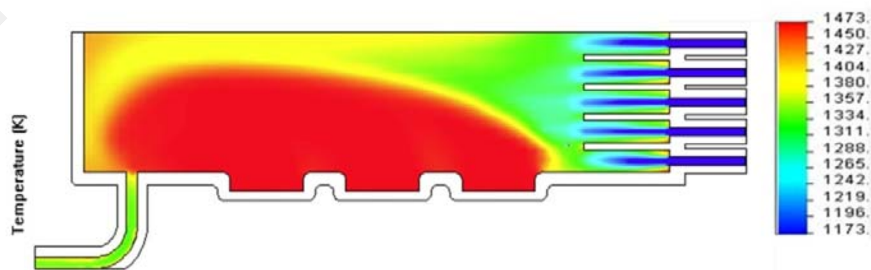

Figure 4.4 Final Temperature Distribution at 1473K

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The simulation results with the inlet fluid temperature of 1473K (1200°C) could be observed in the figure 4.4. 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 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 colour surrounding the chamber, It can be seen in the result where the contour of the colour 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 dark red around the substrate after 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 1473K is not suitable and could turn in to dangerous cases if it is involved with the growth chamber later on.

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4.3.2 Simulation Results at 1373K

Gas temperature features as well as the velocity characteristics obtained from the simulation results are investigated stage by stage for 1373 K temperature. For the initial results, the temperature and velocity occur at initial temperature and velocity at iteration 591 and within 7 hours of first period as shown in figure 4.5. The red colour contour is

manifesting the high temperature, mainly at nozzle inlets and later changes in to other quantified colour contours till the lowest temperature. From the figures with colour 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.

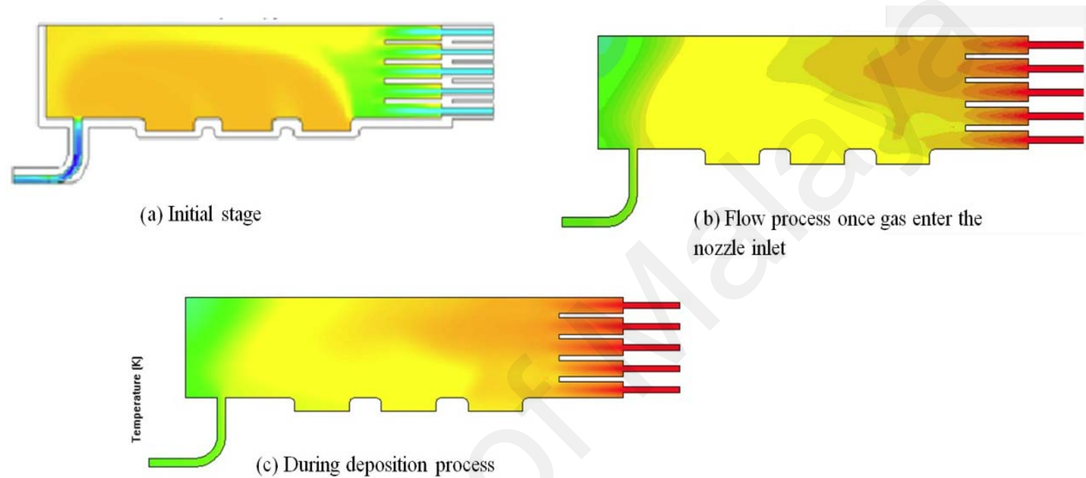

Figure 4.5 Captured figures 1373K temperature distribution

For the first stage as seen in figure 4.5 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.

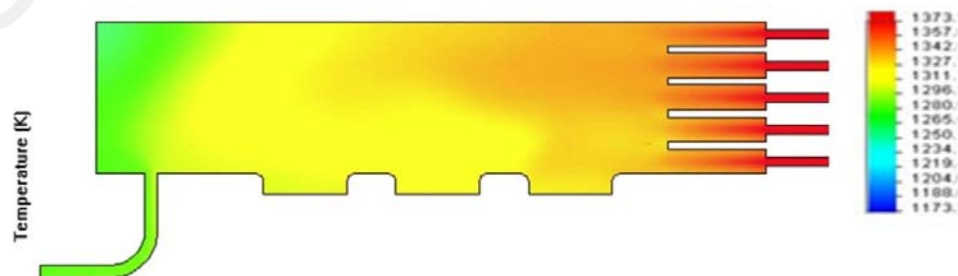

Figure 4.6 : The temperature flow characteristic at 1373K

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This condition occur because at the first gas nitrogen and NH3 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. There is a possibility of mixing up of the liquid within gaps and the growth chamber as shown in figure 4.7.

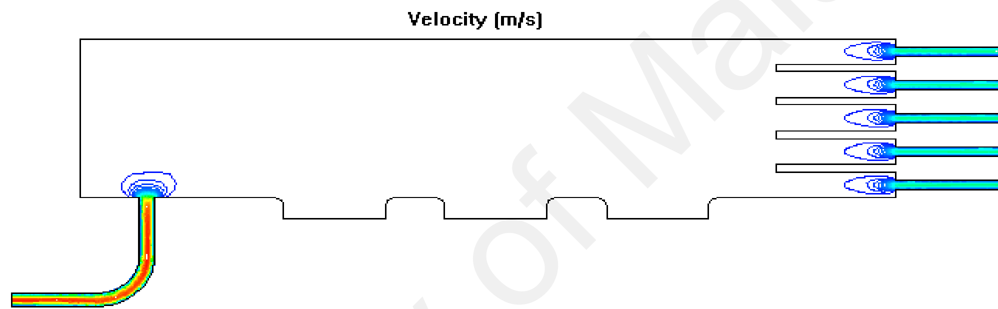

Figure 4.7 : Flow pattern with possible mix liquid between gaps

4.3.3 Simulation Results at 1273K

After certain period of time, captured figures were observed for stage by stage. The final analysis of the gas flow and temperature are shown after few hours as in figure 4.8. Here it has been found out that stability establishes inside and it is finalized by the simulation results. 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.

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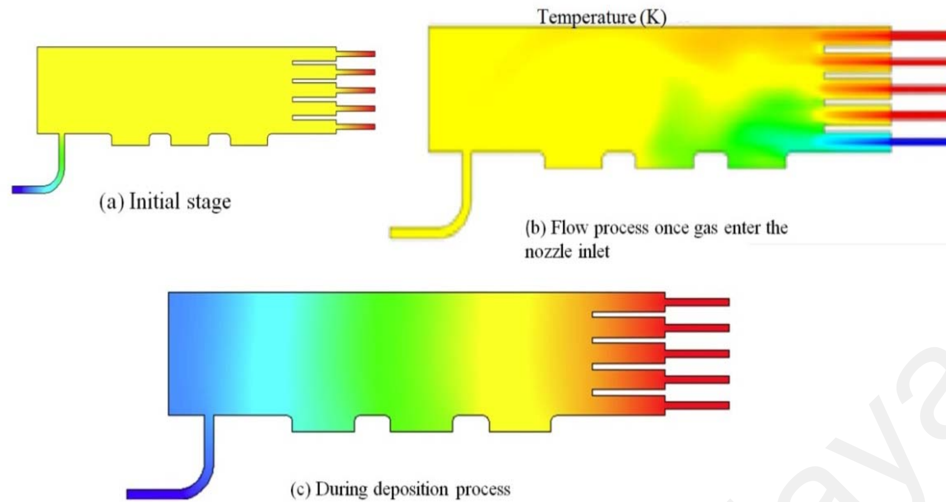

Figure 4.8 Captured figures of 1273K temperature distribution

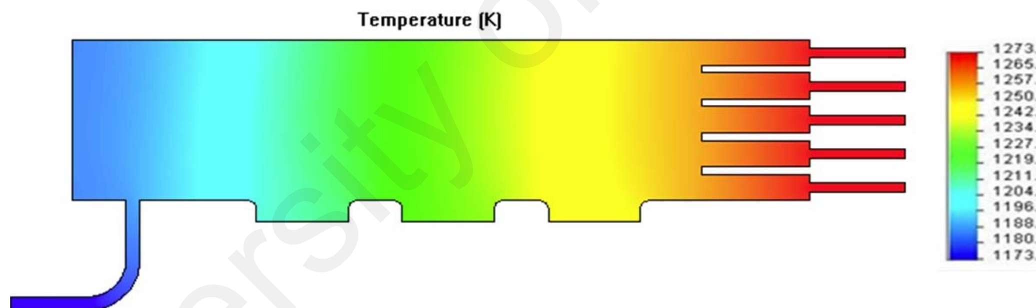

Figure 4.9 Final stage temperature Analysis on 1273K

After reached 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 1273K as in figure 4.9. 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.

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Figure 4.10 shows the data for 1473K-1273K temperature distribution in the MOHVPE reaction chamber model versus different substrate position in 3 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 1473K – 1273K. The first node at 1473K indicates the highest temperature along the chamber from inlet to the holder positions.

The second line 1373K 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 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 1273K range is the most convenient area as observed at substrate holders positions with respect at between 35cm distance from the inlet where the substrate B is located.

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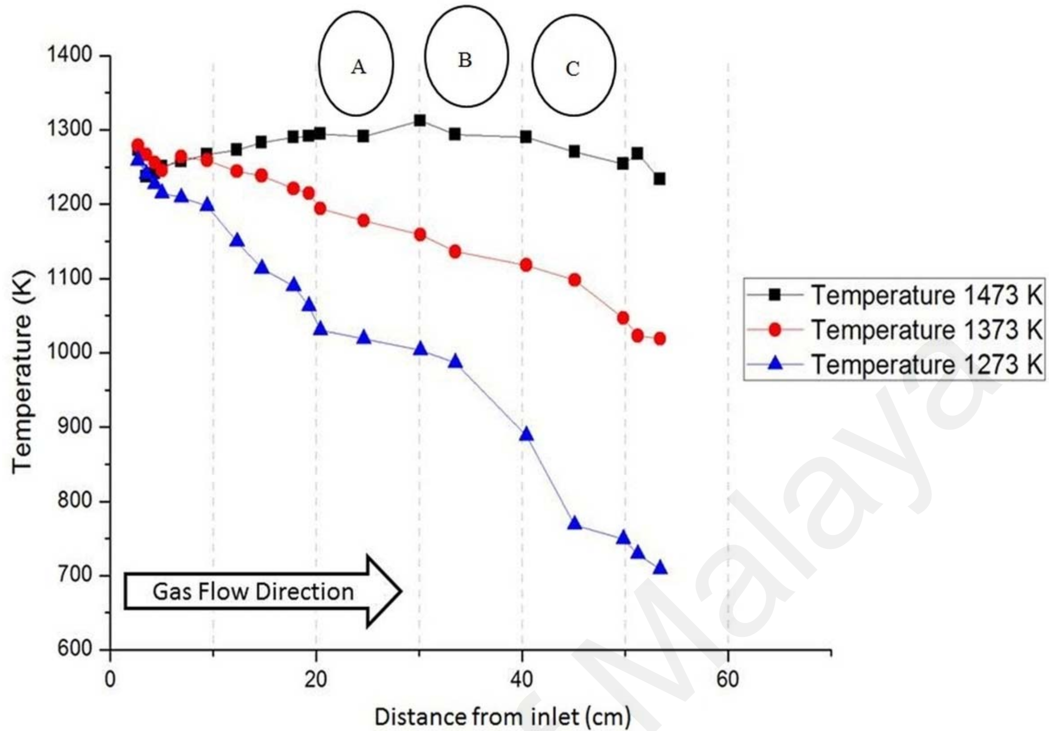

Figure 4.10: Environment achieved an excellent temperature distribution along the chamber

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 1273K 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 1273K is the best performance flow once the gases enter with velocity 0.5m/s to stable up the flow inside the chamber. The uniformity of temperature to stabilize the wafer ranges from 1273K to 1050K at B position (figure 4.10) clarified the best development of the wafer growth at middle holder.

From the graph plot (figure 4.10) it can premixed between NH_3 gas and temperature along the chamber prior to the deposition zone which is substrate holder B

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results in uniform temperature rate profile compared to other holders which are A and C. The different positions of holders from simulation results will influence the growth rate in future research analysis. These conditions of the chamber are supported strongly by the temperature that needs to be synchronized together to produce optimum flow pattern inside the chamber. Based on the basic fundamentals of MOCVD processes, horizontal duct reactors operated at atmospheric or slightly reduced pressures have always been at the centre of interest. The air travels along the five individual paths of five different gaps as a result of such mixing in-between gas. The simplest form reactor is a horizontal rectangular duct type, typically a few centimetres wide and high and a few decimetres long. The inlet and outlet are often thick and shaped to create a smooth transition from reactor's chamber to inlet and outlet tubes. The gases flow out through the outflow plane in horizontal direction. This outlet is located sufficiently far away from the inlet nozzles. During HVPE process the carrier gases used are N_2 and NH_3 where both the gases influence the higher growth rate.

4.4 Gravity and Chamber Length on Temperature inside the chamber

The design criteria of the reaction chamber are mostly established on the empirical experience and profound knowledge about the requirement of processes. Realizing the fluid flow as well as the chemical phenomena occurring inside the reactor and projecting reactor's performance necessitates the capacity of modelling the complexities in chemical kinetics, fluid mechanics and transport phenomena inside the process chamber.

Gravity is one of the important parameters that influence the flow patterns, therefore, growth rate as well as uniformness in the MOHVPE reactor. Gravity just does not engender non uniform films it creates recirculation in to the fluid flow pattern that also leads to memory effect. But if the wafer's film non uniformity is to be meliorated

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and sharp interfaces are to be obtained despite the existence of recirculation, the effect of gravity for both types (vertical and inverted) of reactors have different situation with absence gravity in figure 4.12, that potential exist if films are grown in space of chamber as its driving the flow when there are large differences in density between carrier gas and growth species: a second important parameter is the diffusion coefficient.

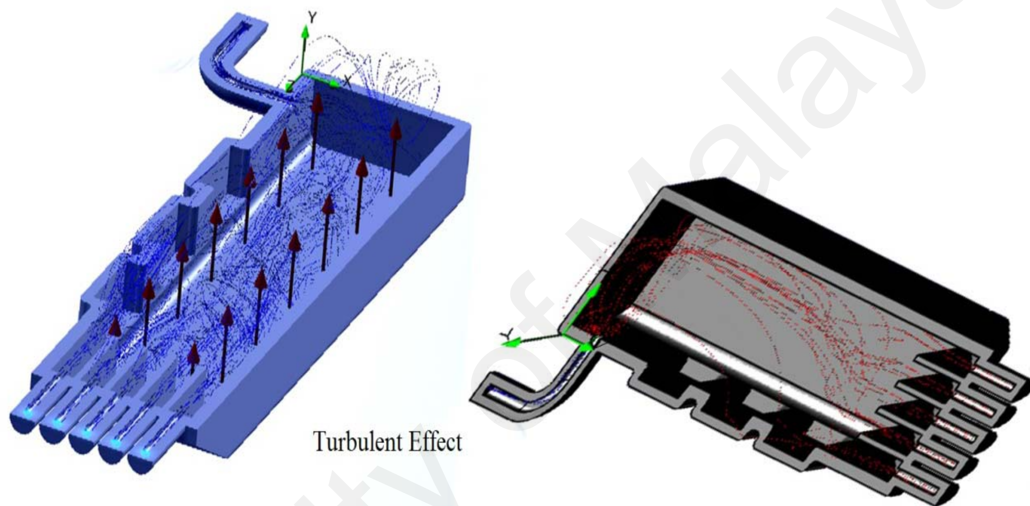

Figure 4.11 : The effect of gravity on geometry in spite of circulation

Simulations of reactor were performed without any reaction to determine the most acceptable geometry subjected to achieve the coveted III/V ratio at 5 inlets of the nozzle. Nitrogen and ammonia are found in greater concentration for such optimized geometries in the centre and at the edges of substrates respectively. The primary design furnishes the least concentration of GaCl but prominently the ammonia. Upstream of the susceptor there is usually a cold entrance region. The carrier gases extremely dilute the reactants leading to longer chamber lengths which may boost the mixing of all available gases though uniformity in their densities at the substrates. Those analyses results

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obtained from the simulations must demonstrate the least length of reactor's chamber length as required to obtain the complete mixing of reactants.

4.5 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 3000 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 figure 4.13instead 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.

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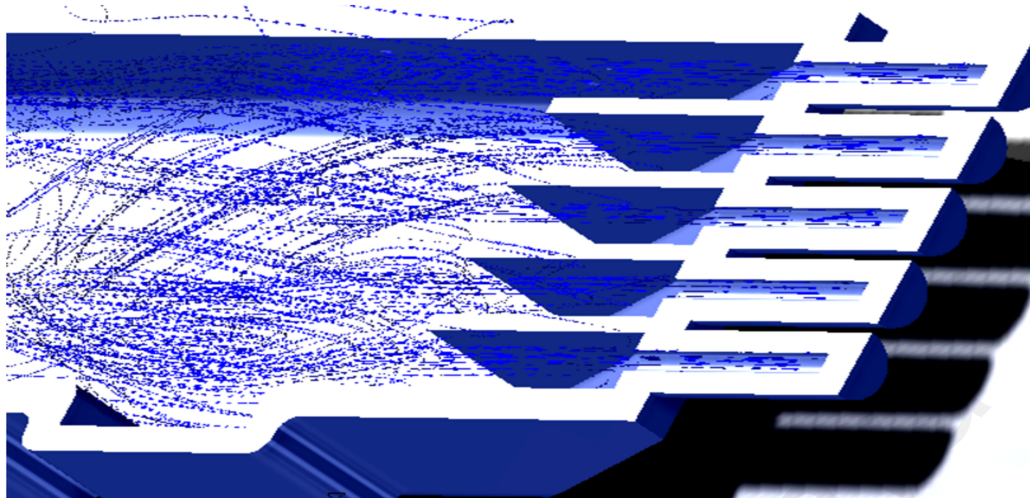

Figure 4.12Turbulent occur at the inlet area after pass the barrier

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 figure 4.14 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.

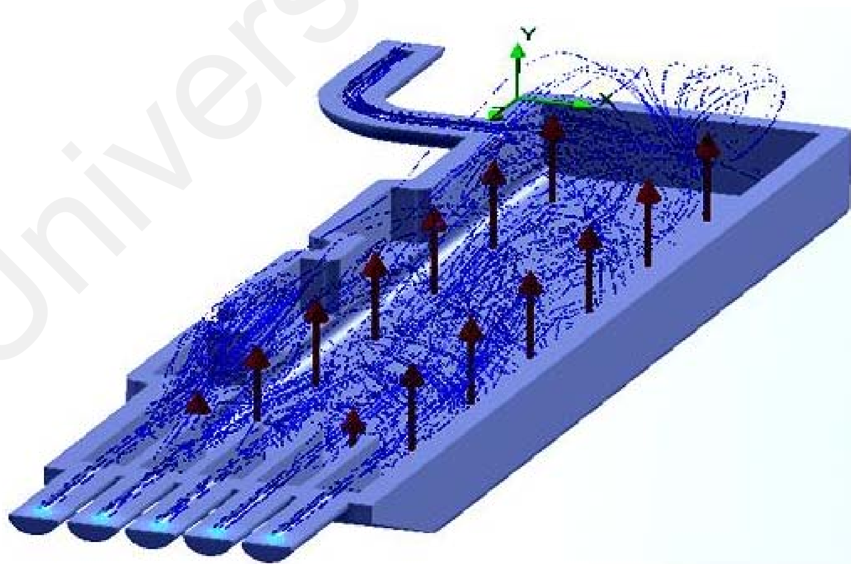

Figure 4.13: Turbulent flow that leads rapidly at inlet nozzle and becomes laminar surrounding the chamber.

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

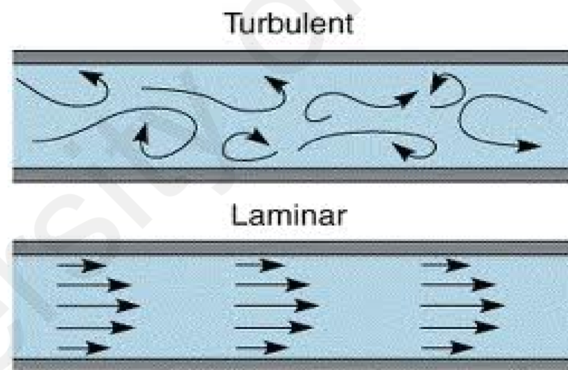

Figure 4.14 : Theoretical turbulent phenomena

Turbulent theory in the figure 4.15 is manifesting the orientation of buoyancy along the x axis, maintaining other parameters unaltered. The appearing velocity of vortex is located very near to the surfaces of the substrate and it is the outcome of gas inflow from the substrate surfaces which is always kept hot. To anticipate the profile of the deposition, an unsophisticated sticking model along with the sticking coefficient is utilized. On the contrary, the regulation chamber for flow of gas works as barrier for

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the ammonia/nitrogen mixture they are forced to maintain a flow (moderately 0.65 m/s) through broad slit upon substrates. The work of observing the turbulence in the simulation shows that the inflow patterns coincide with experimental results while actual growth temperature values are used. Apparently, the flow patterns that turns in to a circle from the reactive species and also the overall constituent fractions might alter with the emergence of GaN that is well known as parasites at the reactor's walls. In such cases, patterns of the backflow gas flow that tremendously affects the duplicability of surface morphologies as well as the growth rates.

4.6 Effect of velocity influenced the reactor geometry

As shown in figure 4.16, inlet flow velocity might be affecting the gases' mean flow rate in to the chamber. Initially, the inlet flow velocityas well as the boundary conditions, Maximum velocity has been detected at the inlet that engendered turbulence in the flow.

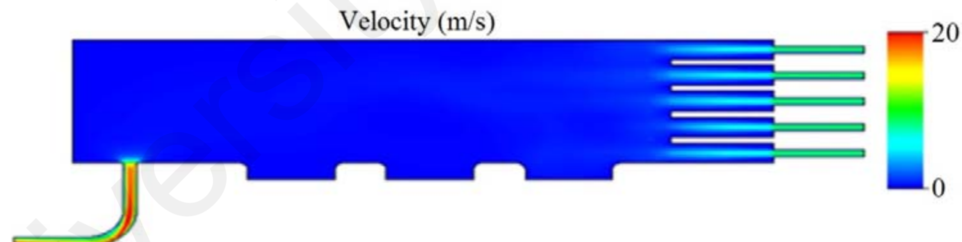

Figure 4.15 Flow pattern of velocity inside the chamber

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The flow characteristics of the gases control the classification of the reaction chamber and it is regarded as one of the most critical subsystems and therefore, precision control system should be installed. This is due to the rate of reaction's direct relationship to their compositions. The result manifests occurrence of turbulent flow over all temperature variations. This is due to shortening of the inlets as well as that of

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the outlet of the reaction chamber in which this short lengths influence the flow to be reversed. To resolve such issues, a newly modified design of the reaction chamber's length might facilitate improved performance; prominently the length increasing of the inlets could reduce the effect of jet. Table 4.1A-4.1C below indicates the detail parameter for velocity.

Table 4.1 (A)Linear flow velocities for inlet gas T=1473K

Goal Name	Averaged Value	Maximum Value
Min Temperature of Fluid	1173.2	1173.2
Max Temperature of Fluid	1473.2	1473.2
Max Velocity	0.84	0.80
Iterations: 9250		

Table 4.1 (B)Linear flow velocities for inlet gas T=1373K

Goal Name	Averaged Value	Maximum Value
Min Temperature of Fluid	1173.2	1173.2
Max Temperature of Fluid	1373.2	1373.2
Max Velocity	0.81	0.65
Iterations:1324		

Table 4.1 (C)Linear flow velocities for inlet gas T=1273K

Goal Name	Averaged Value	Maximum Value
Min Temperature of Fluid	1103.2	1173.2
Max Temperature of Fluid	1273.2	1273.2
Max Velocity	0.60	0.5
Iterations:1486		

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4.7 Pressure at 1273K influenced the reactor geometry

It was observed that in horizontal flow results in a very small change in pressure as high accuracy can hardly be achieved in estimating the residence time. When the temperature is increased the pressure is increased as the higher temperature causes the particles of gases to movement, thus they should make collision against the container's walls(figure 4.18). The flow through the orifice plate increases because of the restriction, and the pressure decreases correspondingly. That is how flow is measured using pressure drop thru the orifice. Square root of dP and pressure-temp compensation gives a desired flow. The reference value of the static pressure is the of the uninterrupted free-stream flow of fluids. Therefore, any fluctuation in the static pressure inside of the tube would be greater or lesser in value than ambience static condition. Holes could be drilled into the walls of the Venturi tube so that the static pressure is measurable. These holes are known as "static taps" and are linked to a "U-tube manometer"—a tube having a U-shape with a liquid such as coloured alcohol within it. When the static pressure is measured at the static tap equals the free-stream static pressure, the fluid levels in the tube are at some equal reference level. But static pressures above or below the free-stream pressure are indicated by a decrease or increase in the level of fluid in the tube.

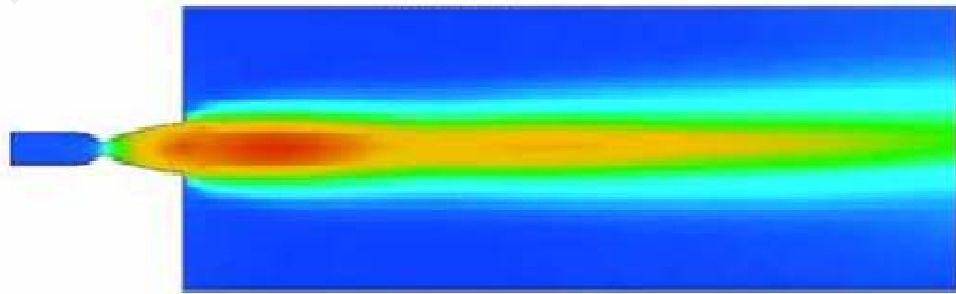

Figure 4.16Pressure over flow process

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The pressure inside the chamber is maintained within it and this remains till the outlet. When the pressure is increased the gas is contracted whereas the reduction of pressure causes the gas to experience expansion. When the chamber volume is holding constant the increased volume resulting from high pressure causes the temperature to be increased and vice versa. But when the volume is not considered as fixed temperature variations causes the gas volume to be altered, i.e. increased temperature leads to gas expansion and vice versa.

4.8 Comparison parameters based on previous result between MOHVPE, HVPE and MOCVD

ITEM	MOHVPE	HVPE	MOCVD
TEMPERATURE	1000°C-1100°C	1300°C-1400°C	1400°C-1500°C
PRESSURE	0.1 Mpa	0.1 Mpa	0.1 Mpa
GAS FLOW	0.01m/s(100m/hour)	0.07m/s(100Nm/hour)	0.03m/s(100Nm/hour)
COST	Low cost	High cost	High cost
GEOMETRY	Horizontal direction	Vertical	Vertical/horizontal
VELOCITY	0.05m/s	0.075m/s	0.075m/s
GROWTH RATE	Low growth rate	High growth rate	High growth rate
FILM LAYER	Thin film	Thick film	Thick film

Table 4. 1 Comparison parameters between previous analysis.

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CHAPTER 5: CONCLUSION AND RECOMMENDATION

5.1 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

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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

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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.

5.2 Recommendation

There are several recommendations in order to improve and for future research as follow:

1) Gain more data about the properties of materials to construct more identical geometry designs of model criterion.
2) Develop the simulation as low cost by using semiconductor simulation to observe the detail of process growth MOHVPE with combination thick and thin layers in single reactor.
3) Finer meshing should be carried out so that the artificial energy in minimized for whole model and thus the accuracy is increased for the results.
4) The simulation show that another important factor for growth rate and flow pattern in horizontal reactors a combination of gravity driven transport and the diffusion coefficient determines the distribution of the growth species.

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CHAPTER 6: REFERENCE AND BIBLIOGRAPHY

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PUBLICATIONS

(1) **N. Zieyana Mohamed Annuar**, Mohd Faizul Mohd Sabri, A. Shuhaimi Abu Bakar Investigation of the Geometry Modeling of Metal Organic Halide Vapor Phase Epitaxy (MOHVPE) Reactor Advanced Materials Research Vols. 626 (2013) 396-400.

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APPENDICES I

```
title MOHVPE simulation

#

# Simulates a simple MODEL device

# Solidworks Design 2012

#--------------------------------------------------------------

# SECTION 1: MESH GENERATION

#--------------------------------------------------------------

#mesh specification


mesh smooth=1 space.mult=1.0

x.mesh l=0.0  spacing=0.5

x.mesh l=2.5  spacing=0.25

x.mesh l=5.0  spacing=0.5

#

y.mesh l=0.0  spacing=0.002

y.mesh l=0.1  spacing=0.002

y.mesh l=3.1  spacing=0.5


#--------------------------------------------------------------

# SECTION 2: REGIONS

#--------------------------------------------------------------

# regions specification


region num=1 Material=GaN   y.max=0.1  emiss.3

region num=2 Material=GaN   y.min=0.1  y.max=3.1    emiss.3
```

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```
elec       num=1  name=anode x.min=2.0 x.max=3.0 y.min=0.0 y.max=0.0

elec       num=2  name=cathode bot


#-------------------------------------------------------------

# SECTION 3: 2D PROFILES

#-------------------------------------------------------------

# specifying Gaussian doping profile


doping   conc=5.0e18   p.type   x.left=2.0   x.right=3.0   gaus   char=0.5
ratio.lat=0.6


#doping profile in particular region


doping uniform region=1 p.type conc=5.0e16

doping uniform region=2 n.type conc=5.0e17

#---------------------------------------------------------------

# SECTION 4: MATERIAL MODELS

#---------------------------------------------------------------

#specifying material parameters


material copt=3e-11

material region=1       taup0=1e-9  taun0=1e-9

material region=2     taup0=1e-9  taun0=1e-9


#specifying model application in each region


model optr srh bgn  kla bbt.kl print

#----------------------------------------------------------------
```

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```
# SECTION 5: OUTPUT
#-----------------------------------------------------------------
#specifying desirable results output for analysis
output con.band val.band recomb u.srh u.aug u.rad band.param
#
#-----------------------------------------------------------------
# SECTION 6: INITIAL SOLUTION
#-----------------------------------------------------------------
# no carriers
solve init
#------------------------------------------------------------------
# SECTION 7: boundary conditions
#------------------------------------------------------------------
# 0.0 to 3.5 V forward bias
log outf=homo01.log master
method newton climit=1e-4 maxtrap=10
solve  l.wave=0.363 vanode=0.0 vstep=0.1 vfinal=3.5 name=anode
save outfile=homo01.str

# structure plot
tonyplot homo01.str -set optoex06_0.set
# radiative recombination rate contours
tonyplot  homo01.str -set optoex06_1.set
# luminous intensity vs bias
tonyplot homo01.log -set optoex06_2.set
#-------------------------------------------------------------------
# SECTION 8: EXTRACTION
#-------------------------------------------------------------------
```


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```
# Extract total and radiative components of recombination

# (can be used to calculate luminous efficiency)

Simulation profile on double heterojunction InGaN based LEDs


mesh smooth=1 space.mult=1.0

x.mesh l=0.0  spacing=0.5

x.mesh l=2.5  spacing=0.25

x.mesh l=5.0  spacing=0.5

#

y.mesh l=0.0  spacing=0.1

y.mesh l=0.5  spacing=0.05

y.mesh l=1.0  spacing=0.002

y.mesh l=1.1  spacing=0.002

y.mesh l=1.6  spacing=0.002

y.mesh l=4.6  spacing=0.5


#eliminate unnecessary bulky region


eliminate y.direction x.min=0.0 x.max=5.0 y.min=3.6  y.max=4.6

#

#-------------------------------------------------------------

measure u.total

measure u.radiative

quit
```

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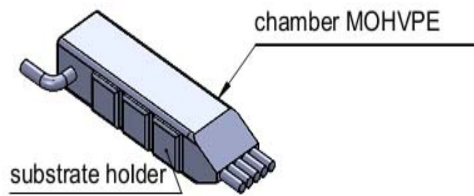
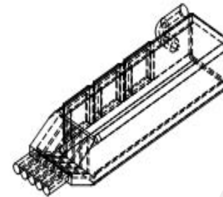
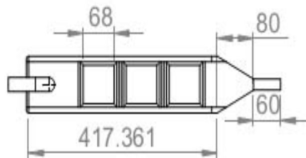
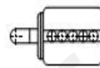
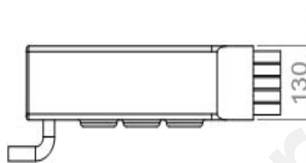
APPENDICES II











CAD DRAWING	GROWTH CHAMBER MOHVPE
NURUL ZIEYANA MOHAMED ANNUAR	DATE: 20HB OCTOBER 2011
DEPT. OF MECHANICAL ENG	UNIV. OF MALAYA

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