Flux profile modelling using numerical methods

Bharat Reddy Pemmireddy
University of Nevada, Las Vegas

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FLUX PROFILE MODELLING USING NUMERICAL METHODS

by

Bharat Reddy Pemmireddy

Bachelor of Engineering
Osmania University, India
2002

A thesis submitted in partial fulfillment
of the requirement for the

Master of Science Degree in Electrical Engineering
Department of Electrical and Computer Engineering
Howard R. Hughes College of Engineering

Graduate College
University of Nevada, Las Vegas
August 2004
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ABSTRACT

Flux Profile Modeling Using Numerical Methods

by

Bharat Reddy Pemmireddy

Dr. Rama Venkat, Examination Committee Chair
Professor and Chair
Department of Electrical Engineering
University of Nevada, Las Vegas.

Molecular beam Epitaxy (MBE) is a physical vapor deposition system, used to grow semiconductor layers (epilayers). In order to increase the economics of MBE, the industry has increased the size and number of wafers processed in one stage. This lead to, non-uniformity in thickness of material grown. In this work a process simulation tool based on numerical methods was developed to study different parameters which affect the thickness. The process of emission in open cells was identified as free evaporation and for computer simulation of these types of cells Model I was developed. The process of emission in closed cells with orifice was identified as Knudsen effusion and for computer simulation of these types of cells Model II was developed. The cosine law of effusion was modified to account for the focusing effect exhibited by the industrial cells. The modified law involves parameter N and as N increases the focusing effect increases. The experimental data for 10,000G SUMO cell are in good agreement with the results of Model II for modifying parameter N=1.9. From the study of different parameters it is

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observed that for the GEN 2000 MBE equipment which use 10,000G SUMO cell, if the angle of tilt is increased from 45° to 52° the flux variation reduces from 3.67% to 0.45%.
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CHAPTER 1

INTRODUCTION

1.1 Deposition Technology

Deposition technology can well be regarded as the major key to the creation of applications such as computers, communication devices and many more. The heart of all these applications is microelectronic solid-state devices which are based on material structures created by thin-film deposition. Electronic engineers have continuously demanded films of improved quality and sophistication for solid-state devices, requiring a rapid evolution of deposition technology. Equipment manufacturers have made successful efforts to meet the requirements for improved and more economical deposition systems. Another important reason for the rapid growth of deposition technology is the improved understanding of the physics and chemistry of films, surfaces, interfaces, and microstructures made possible by the remarkable advances in analytical instrumentation. A better fundamental understanding of materials leads to expanded applications and new designs of devices that incorporate these materials.

The semiconductor industry manufactures thin films from a wide variety of materials by deposition from the gas, vapor, liquid, or solid phase. The process of growing single crystal film on a single crystal substrate of the same crystallographic orientation is known as homoepitaxy. If a single crystal film is deposited on a single crystal substrate of different crystallographic orientation, the process is termed heteroepitaxy. Subsequent
steps in the fabrication process create electrical structures that require the deposition of an insulating or dielectric layer, such as an oxide, glass, or nitride. Film formation by methods other than deposition are used in a few steps of the fabrication sequence; these include thermal oxidation of the substrate, ion implantation, nitridation, silicide formation, electrolytic and electroless metal deposition, and spray deposition (e.g., of organometallic solutions for forming antireflection coatings).

1.2 Classification of deposition systems

There are many dozens of deposition technologies for material formation. Since the concern here is with thin-film deposition methods for forming layers in the thickness range of a few nanometers to about ten micrometers, the task of classifying the technologies is made simpler by limiting the number of technologies to be considered. A survey of thin film deposition technologies is provided in the Appendix. Basically, thin-film deposition technologies are either purely physical, such as evaporative methods, or purely chemical, such as gas and liquid phase chemical processes. A considerable number of processes that are based on glow discharges and reactive sputtering combine both physical and chemical reactions; these overlapping processes can be categorized as physical-chemical methods. The explanation of individual processes is beyond the scope of the work and hence the reader is referred to any standard text book on deposition techniques [1-4].
1.3 Molecular Beam Epitaxy (MBE)

MBE [5-7] is a sophisticated, finely controlled method for growing single-crystal epitaxial films in a high vacuum (10\(^{-11}\) torr). The films are formed on single-crystal substrates by slowly evaporating the elemental or molecular constituents of the film from separate Knudsen effusion source cells (deep crucibles in furnaces with cooled shrouds) onto substrates held at a temperature appropriate for chemical reaction, epitaxy, and re-evaporation of excess reactants. The furnaces produce atomic or molecular beams of relatively small diameter, which are directed at the heated substrate, usually silicon or gallium arsenide. Fast shutters are interposed between the sources and the substrates. By controlling these shutters, one can grow superlattices with precisely controlled uniformity, lattice match, composition, dopant concentrations, thicknesses, and interfaces down to the level of atomic layers.

The most widely studied materials are epitaxial layers of III-V semiconductor compounds, but silicon, metals, silicides, and insulators can also be deposited as single crystal films by this versatile and uniquely precise method. Complex layer structures and superlattices for fabricating gallium arsenide heterojunction solid-state lasers, discrete microwave devices, optoelectronic devices, waveguides, monolithic integrated optic circuits, and totally new devices, have been created. An additional important advantage of MBE is the low temperature requirement for epitaxy, which for silicon is in the range of 400°C to 800°C, [6] and for gallium arsenide, 500°C to 600°C [6]. Several production systems with associated analytic equipment are now available [7]. In the following paragraphs a brief explanation of components involved in MBE is provided.
1.4 Overview of MBE system

The whole MBE process can be divided into three stages, wafer preparation, deposition and characterization. Each stage and the associated modules are shown in Figure 1.1 and 1.2. A brief discussion of each of the stages is presented below.

1.4.1 Wafer Preparation

Wafers or substrate are placed in a cassette holder and the holder is loaded into a cassette rapid entry lock system. The cassette is then moved to preparation chamber in which the oxides on the wafer are removed by heating. In the same chamber, the wafer is treated to remove the defect density so as to grow good quality layers. The preparation chamber is equipped with analytical tools such as Reflection High Energy Electron Diffraction (REEHD), Auger Electron microscopy (AES) etc. to study the surface of the wafers before and after deposition. These analytical tools will be discussed in a separate section.

1.4.2 Deposition Chamber

The process of deposition is carried out in the deposition chamber. Due to the stringent requirement of purity of the epilayers, the environment in which it is grown should be ultra clean. This is ensured by pumping the chamber to ultra high vacuum (UHV) which is usually to the order of $5 \times 10^{-11}$ torr. To reduce contamination from vacuum systems oil free pumps such as cryo or turbo pumps, are used as main pumps and ion or sublimation pumps are used as supplements. Cryo paneling is done inside the chamber to reduce cross talk between source cells and also to maintain the UHV environment. The wafer is fixed on a substrate manipulator which provides X, Y and Z movements to the wafer. The manipulator provides continuous azimuthal rotation to the
wafer and can also be adjusted to change the source to substrate angle. Ion gauge is provided on the manipulator for pressure measurements in the chamber. Ports are provided in the chamber to house growth monitoring facilities and introduce source cells. Layers of different composition can be grown by controlling the molecular beams from source cells containing different materials. Molecular beams are controlled by a combination of shutters located near the openings of the cell and also a single shutter located at the wafer.

1.5 Measurement Techniques in MBE

Almost all modern MBE equipment has special ports which provide access for in-situ monitoring and analysis. As reproducibility is of major concern these facilities allow monitoring of growth conditions, and accurately control growth parameters. In the following sections a brief introduction to these techniques are provided

1.5.1 Reflection High Energy Electron Diffraction (REEHD)

RHEED [8] is a simple and robust tool which can give qualitative measurements in surface analysis. The principle of RHEED involves directing a high energy beam of electrons on to the wafer and collecting the reflected electrons on a phosphorous screen located in the deposition chamber. The beam is produced by RHEED gun and its energy is usually 10keV. The electrons interact with the periodic potential of the crystalline material grown on wafer and get scattered. The scattered electrons when collected on the screen form a diffraction pattern, whose sharpness of the pattern depends on the periodicity of the crystal.
RHEED is particularly suitable for MBE because the RHEED Gun and the phosphorus screen are located on either side of the wafer and hence do not obstruct the molecular beam coming from the source cell. In MBE, RHEED is used to monitor the crystallinity, the crystal structure and lattice parameters of the material grown. In modern MBE system, RHEED has become standard equipment.

1.5.2 Ellipsometry

Ellipsometry [9] is an optical characterization technique used to measure layer thickness uniformity and composition. In this technique, a linearly polarized monochromatic light is incident on the wafer. The reflected light changes its polarization from linear to elliptical. The change in polarization is measured by two parameters \( \Delta \) and \( \Psi \). The parameters \( \Delta \) and \( \Psi \) directly measure the degree of ellipticity of the reflected light and indirectly yield the film thickness.

Ellipsometry was introduced into MBE following the work of Demay et. al [10]. Demay et. al [10] have fitted the ellipsometry equipment into one of the ports provided in standard MBE system. They studied initial growth parameters by plotting \( \Delta \) and \( \Psi \) V/s time and parametrizing the plots. They also obtained compositions by converting the ellipsometry data to dielectric function of the layer and fitting the function to existing theoretical model to calculate composition. Ellipsometry is a non destructive technique. It is experimentally easy to conduct and gives highly precise values.

1.5.3 Auger Electron Microscopy (AES)

AES [11] is a technique to identify the type of elements present and also their concentration. The general principle involves an electron energetic beam which excites the core electrons to higher states and when these energetic electrons jump into lower
state they impart their energy to other electrons which are, then, released with a well
defined energy characteristic of the atom. The beam is produced by an electron gun and
its energy ranges within 2-25keV. When the excited electrons jump to lower states, they
do so by either releasing their energy as photon or transferring its energy to other
electrons in same or different states. The probability of latter process occurring is higher
for lighter elements. The released electron is called Auger electron and its energy
characterizes the parent atom.

AES can be used to map the distribution of elements on a surface. It can also be
combined with ion beam etching to give depth profiles. In MBE, it is used to monitor the
composition of the epilayer and is limited to analysis on few atomic layers on the wafer.

1.5.4 Quartz Crystal Monitor (QCM)

In MBE, QCM [12] is used to measure deposition rates at any location on the wafer.
QCM consists of piezoelectric material like quartz to which an AC voltage is applied,
because of the piezoelectric property of the crystal, it responds to the AC voltage by
producing an AC current with fixed frequency. When the mass of the material deposited
is small the change in frequency of oscillation of the current is directly proportional to the
change in mass of material deposited. The formula to calculate thickness \( t \) is given by:

\[
\rho_t t = \left( \frac{\rho_q t_q}{f_q} \right) (f_c - f_q)
\]  

(1.1)

where \( \rho_t \) is density of material deposited, \( \rho_q \) is density of quartz crystal, \( t_q \) is thickness
of quartz crystal, \( f_q \) is resonant frequency of quartz crystal and \( f_c \) is resonant frequency of
quartz crystal with material deposited on it. In MBE, QCM is mounted on one end of the
arm whose other end is free to rotate, the movement of the arm is computer controlled.
The crystal is initially positioned at the center of the chamber (center of the wafer) and
moved in predetermined steps towards the edge of the wafer. At each step the deposition rate is calculated and plotted against the position of the crystal which provides the spatial flux profile at the wafer.

1.5.5 X-Ray Diffraction (XRD)

X-rays [13] are electromagnetic radiation with typical photon energies in the range of 100 eV - 100 keV. For diffraction applications, only short wavelength X-rays (hard X-rays) in the range of a few angstroms to 0.1 angstrom (1 keV - 120 keV) are used. Because the wavelength of X-rays is comparable to the size of atoms, they are ideally suited for probing the structural arrangement of atoms and molecules in a wide range of materials. The energetic X-rays can penetrate deep into the materials and provide information about the bulk structure. X-ray diffraction analysis is nondestructive and the conventional setup is relatively cheap.

When x-rays are scattered from a crystal lattice, constructive interference occurs and when Bragg's Law [13] is met:

$$2d \sin \theta = n\lambda$$

(1.2)

where, $\lambda$ is the wavelength of the X-ray. $\theta$ is known as diffraction angle, and it is the angle between incident beam and the diffracted beam; $d$ is the spacing of the reflection planes (not necessary the planes parallel to surface). Equation 1.2 allows us to calculate details about the crystal structure.

Usually there are two scanning modes for X-ray diffraction analysis: $\theta$-$2\theta$ (normal scan) and $\Omega$ scan (rocking curve). During $\theta$-$2\theta$ scan, the X-ray source and the detector are rotated and the sample is not moved. $\Omega$ is the angle which lies in the plane of the sample and in $\Omega$ scan, only the sample is rotated.
Basic XRD measurements made on thin film samples include:

- Precise lattice constants measurements derived from $\theta - 2\theta$ scans, which provide information about lattice mismatch between the film and the substrate and therefore is indicative of strain & stress

- Rocking curve measurements made by doing a $\theta$ scan at a fixed $2\theta$ angle, the width of which is inversely proportionally to the dislocation density in the film and is therefore used as a gauge of the quality of the film.

- Superlattice measurements in multilayered heteroepitaxial structures, which manifest as satellite peaks surrounding the main diffraction peak from the film. Film thickness and quality can be deduced from the data.

- Glancing incidence x-ray reflectivity measurements, which can determine the thickness, roughness, and density of the film. This technique does not require crystalline film and works even with amorphous materials.

The layer thickness can be determined from the thickness fringes formed in the rocking curves. The formation of thickness fringes involves complicated dynamical theory and is beyond the scope of this work, for a complete description the reader is referred to Schuster and Herres. [14]

1.6 Types of Knudsen Cells

The design of source cells is crucial in deciding the flux uniformity at the wafer and efficiency of use of the material. The uniformity in thickness of material deposited at various locations on the wafer depends on the flux of molecules arriving at those locations. The flux on wafer largely depends on orientation of cell to wafer in terms of
distances and angles and in most of the industrial MBE systems these parameters are fixed and hence, the geometry of cell used plays a crucial role in deciding the uniformity of film thickness. Another important parameter is efficiency which is defined as the ratio of material put out of cell to the material actually deposited on the wafer. Since the materials used in MBE process are ultra pure and hence very expensive and hence, efficiency is an important parameter. Efficiency is quite low for the present cells used in industrial MBE and can be improved largely by a good cell design. The cells are classified according to the states of sources used in the cell as Solid Source and Gaseous Source MBE cells.

1.6.1 Solid Source MBE cells (SSMBE)

In SSMBE, [15] the material to be deposited is contained in an inert cell in the solid state. The material is heated by radiation from a resistance heated source. At sufficiently high temperatures the material is evaporated and directed as molecular beams towards the wafer. Heating is provided by spirally wound resistor made of refractory materials like Ta around the cell. The temperature of the cell is controlled by thermocouples. In modern cells the temperature can be gradually varied across the length of the cell. In some cases, as the deposition process is in progress the effective radius of opening of the cell reduces as the material condenses on it, which causes a shift in the flux profile. Shifts in flux profiles leads to poor reproducibility of films and it can be avoided by maintaining the opening of the cell at higher temperatures to remove condensation. The cells employed should be able to withstand high temperatures (up to 1400°C) and should not incorporate any impurities into the beam. Nowadays, cells made out of Pyrolytic Boron Nitride (PBN) are used which have the desired characteristics.
For applications which need dimeric arsenic (As₂) extra attachments to regular cell are needed because As₂ cannot be formed by normal evaporation. As₂ is obtained by separating or cracking tetrameric arsenic (As₄) and for this purpose, a cracker cell is employed. A cracker cell consists of two regions, one in which arsenic is evaporated to form As₄ and a second baffled region, which is maintained at higher temperature allowing multiple collisions of As₄ to split it into As₂.

1.6.2 Gas Source MBE cells

In fabricating most of the optoelectronic devices, Phosphorous (P) is frequently encountered. In SSMBE, it is difficult to obtain quality phosphorous based materials such as InP or their heterostructures because the effusion sources rapidly deplete the source and they are unable to control the P concentration. GSMBE [15] solves the problem by cracking the P series from the gas phosphine (PH₃.) The cracking can be done at high or low pressures. High pressure source gases are used for group V materials and low pressure gas sources are used for group III metal organics. The thickness of the material deposited depends on the deposition rates and substrate temperature. The problem with GSMBE lies in the handling of gases like PH₃ and AsH₃ which are highly poisonous.

1.7 MBE in research

Using sophisticated MBE growth, lithographic and etching techniques it is possible to fabricate new forms of active device with 'tailor made' characteristics [16]. Some of the more significant physical characteristics of the structures observed thus far are indicated in the following paragraphs.
1.7.1 The modulation doped heterostructure

The concept of selective doping in heterostructures, frequently called modulation doping, has been demonstrated in structures designed to separate mobile carriers from their parent impurities. A layer of aluminum gallium arsenide (Al\textsubscript{x}Ga\textsubscript{1-x}As) as grown on gallium arsenide (GaAs) is an example of such a structure. In this example, electrons from donors in Al\textsubscript{x}Ga\textsubscript{1-x}As move to the GaAs leaving behind ionized donors. The separation of the negative electrons from the positive donors sets up an electric field which confines electrons within 100 Å of the interface but leaves them free to move parallel to it. These confined electrons are known as a two-dimensional electron gas (2DEG) which has a number of interesting properties. One such property is an electron mobility which can be considerably greater than that of the bulk GaAs. This is because the electrons are spatially separated from their parent donors.

The mobility can even be further enhanced by growing an undoped Al\textsubscript{x}Ga\textsubscript{1-x}As layer, a so called spacer, in between doped Al\textsubscript{x}Ga\textsubscript{1-x}As and the undoped GaAs. The enhancement in electron transport properties is especially marked when the structures are cooled to cryogenic temperature. Electron mobility exceeding 10 million cm\textsuperscript{2} /V. s at low temperatures (-0.35 K) have been reported. This is over 2000 times higher than in conventional GaAs. This fact makes an Al\textsubscript{x}Ga\textsubscript{1-x}As -GaAs heterostructure very suitable for high speed electronic devices. The high electron mobility transistor (HEMT), also known as a modulation-doped field effect transistor (MODFET), is an example of an application of this heterostructure. The HEMT which operates at high frequencies is becoming the transistor of choice for millimeter wave and high speed applications. For
example, the HEMT is used in radio astronomy and many millions of these devices are produced annually for the low noise front-end of satellite TV receivers.

Also at LSI level of complexity HEMT technology has shown excellent speed performance. A 64 kbit static RAM with an address access time of 1.2 ns and 45 k gate array with 35 ps logic delay have been achieved at room temperature; both of these are the fastest circuit operations ever reported. These complexities are a critical threshold in making HEMT technology practical in future high-speed computer and communication systems. Performance can be further enhanced by including a strained InGaAs channel between the AlGaAs and GaAs layers to make a second generation pseudomorphic HEMT. This is because InGaAs has a higher conduction band discontinuity of 0.3 eV and very high sheet carriers of up to $4 \times 10^{12} \text{ cm}^{-2}$ with no persistent photoconductivity.

In the academic world, wider scientific interest has tended to concentrate on low temperature and strong magnetic fields electronic studies of 2DEG. In high quality modulation-doped AlGaAs/GaAs heterostructures exciting physical characteristics were observed such as the fractional quantum Hall effect [17] and Wigner crystallization [18]. Studies of quantum point contacts have also relied upon this system.

1.7.2 Quantum cascade laser

Recently, researchers at the AT&T Bell Laboratories reported the design and demonstration of a new injection laser using MBE and band structure engineering. The so-called quantum cascade laser [19] is fundamentally different from diode lasers. In conventional diode lasers, the photons emerge from the recombination of electrons and holes, while in quantum cascade lasers, the photons are emitted as electron cascade from one energy level down to another in a staircase-like arrangement of quantum wells. It
operates like an electronic waterfall. This laser relies on only one type of carrier, i.e. electrons and therefore, it is unipolar. The wavelength of the emitted light can be tuned by simply changing the thickness of the quantum wells. However, the layer thicknesses have to be controlled precisely to atomic dimensions, which can be achieved by probably, MBE only. The wavelength can be tailored from the mid-infrared to the sub millimeter wave region in the same heterostructure material. The potential applications for quantum cascade lasers are different from those of conventional semiconductor lasers which are used in compact disk players and light wave communications. Quantum cascade lasers are expected to be used in environmental and industrial process control.

1.7.3 Quantum wires and boxes

The creation and investigation of semiconductor quantum dot (QD) and quantum wire (QWR) structures are in the focus of the work of many leading semiconductor laboratories because of their anticipated novel properties. While quantum wells structures are widely used in optoelectronic devices, QWR’s and QD’s appear to be more difficult to fabricate for this application.

Several methods were proposed for the fabrication of QWRs and QDs by MBE including patterning of 2D heterostructures, growth on stepped and corrugated surfaces, and growth in V-grooves. One of the most promising methods to create QWR’s and QD’s structures is using a strain induced self organized growth process. This method gives the unique possibility to create dense arrays of isolated QD’s with dimensions lower than exciton Bohr radius. The 3D nucleation of InAs above certain coverage has been shown to produce InAs islands having an individual size compatible with quantum confinement, and having a narrow size distribution.
Researchers around the world are very active in this QWR and QD self organization area for the purpose of fabricating quantum wire and dot lasers. QD lasers are thought of to revolutionize the design and application of semiconductor injection lasers, light emitting diodes and light modulators. The interest in QWR or QD lasers is caused by the possibility of modifying the density of states of the active media. Several parameters are expected to be enhanced such as temperature stability of threshold current, modulation bandwidth, and differential gain. In addition, in QD lasers the surface recombination on facets occurring in stripe laser is avoided resulting in higher efficiencies and lower degradation rate.

Recently, an in-situ MBE growth method for the fabrication of QWR’s has been demonstrated [20]. In this method, called cleaved-edge overgrowth (CEO), layers are grown on the natural cleavage plane of an already grown (100) oriented wafer. Present QWR fabrication technology is limited by the wire widths of several hundred angstroms and imposes a considerable variability on the wire width. The CEO technique has been shown to be able to generate atomically precise QWR’s with minimum fluctuation of the wire width. Recently, CEO has led to a demonstration at 4K of a low-threshold current injection quantum wire laser based on electron-hole recombination at intersecting quantum wells.

1.8 MBE as a production epitaxial technology

The demands on an MBE system in a production environment are more stringent than a research machine because of the need to maintain consistent specifications on wafers of a given material structure. In an epitaxial production based operation the most important
parameters are high throughput, uniformity in layer thickness, doping and composition profiles, low surface defect density, large wafer area, long up-time, and versatility. All these major factors are responsible for the sustained success of MBE as a growth technique for electronic and optoelectronic devices.

1.8.1 Production of MMIC’s and HBT’s

In the mass production of Microwave Monolithic Integrated Circuit’s (MMIC’s) and high power Heterojunction Bipolar Transistor’s (HBT’s) with many emitter fingers fabrication, it is necessary to control the defect density which dominates direct performance such as breakdown voltage of Metal-Insulator-Metal (MIM) capacitors for MMIC’s. A low surface defect density of less than 10 cm\(^2\) is now routinely achieved. These defects also cause the processing difficulty to be compatible with fine-line lithography. The MBE growth chemistry is relatively simple, and this facilitates the fabrication of many different types of epitaxial profiles and improves the reproducibility of layer compositions, which is important both in industrial and research environments where wafers of different structures have to be grown. The source materials are relatively pure and less poisonous, and therefore reducing the number of variables influencing material quality and making the operation safer.

In order to achieve greater productivity, the semiconductor industry has consistently increased the size of wafer every few years. This will present a major opportunity for fundamental change in the design and construction of manufacturing equipment and facilities. However, the wafer size will be crucial to the industry productivity, and indeed profitability, in the following decade. Machine up-time is an important factor in the throughput of an MBE machine. The reduction in the cost of manufacture for MBE GaAs
wafers and enhancement of the manufacturability of GaAs MBE are continuously improved due to the long up-time. To minimize the machine down-time preventive maintenance schedule and component improvements are being adopted. The component most prone to failure is the continuous azimuthal rotation (CAR) which holds the wafer during growth. This assembly is subjected to considerable mechanical motion in a mass production. Furnace shutters and effusion cells also exhibit failures. In general, the up-time of an MBE machine is about 85%.

The type of MBE devices that are mass produced include, Metal-Semiconductor-Field-Effect-Transistor (MESFET), HEMT, Pseudomorphic HEMT (PHEMT), Planar Doped PHEMT, Lattice matched HEMT (LMHEMT), Pseudomorphic LMHEMT, Planar Doped LMHEMT, edge emitting lasers (780 to 1060 nm), surface emitting lasers (980 nm), Quantum Well Infrared Photodetectors (8-15 pm), and metal-semiconductor-metal (MSM) detectors (1.3-1.5 pm).

1.8.2 Production of GaAs / AlGaAs lasers

Laser diodes have been extensively used in a wide range of optoelectronic applications, including optical communications, compact disks (CDs), video disks (VDs) and laser beam printers. It is estimated that over 7 million laser diodes are produced and sold each month. Approximately 95% of all the different types of laser diodes are AlGaAs laser diodes with wavelengths ranging from 770 to 860 nm. These are mainly used in audio CDs, CD-ROM, optical memories, VDs, laser beam printers and optical measurement equipment.
1.8.3 Production of Hall elements

In recent years, there have been strong demands for Hall elements for the market of electronic equipments such as video cassette recorders, floppy disk drives and CD-ROM drives. In these equipments the Hall elements are mainly used for brushless motors as magnetic sensors. InSb thin film Hall elements and GaAs Hall elements are well-known and are produced in high volume as magnetic field sensors. InSb Hall elements have high sensitivity to the magnetic field but are not suitable for high temperature operation. On the other hand, GaAs Hall elements have good temperature stability but their sensitivity is not so high. Thin film InAs Hall elements were predicted to have both high sensitivity and stability at high temperature operation. However, it is difficult to obtain InAs thin film with submicron thickness, high electron mobility and high sheet resistance required for high sensitivity Hall elements. These problems were solved by employing MBE to grow InAs thin film on GaAs substrates with 0.5 pm thickness and higher electron mobility of more than 10,000 cm$^2 /V.s$ at room temperature.

1.9 Thesis objective

The extremely limited product throughput, the complex operation, and the expensive equipment are, at present, the major limitations of this promising deposition technology for production applications. To face these problems the industry is increasing the number of devices produced in one run (yield) by increasing the size and number of wafers processed in each run. Their attempts have been limited by the uniformity of thickness and concentration of the layer deposited.
Uniformity in thickness is a crucial parameter as many of the electrical properties of devices depend on this parameter. For example, the threshold voltage of a field effect transistor is proportional to the square of the thickness of the layer. The present work is focused on solving some of these problems. The uniformity of thickness and composition on the wafer depends on, the distribution of flux in the molecular beams reaching the wafer from the cell. In this work, the process of formation of molecular beams from a variety of cells is understood. Based on the theory, a computer simulation tool is developed to aid in better design of the Knudsen cells.

1.10 Organization of the thesis

In the next chapter a detailed review of available literature on the deposition process in MBE is provided. The literature review covers, the concepts involved in the formation of molecular beams, earlier work on Knudsen cells and computer models developed to obtain distribution of flux. In chapter 3, the mathematical formulation available to describe the distribution of flux from earlier cells is provided. In this chapter, the modification of the existing formulation for obtaining flux distribution from cells used in present industry is also provided. In chapter 4, a detailed explanation of steps taken in developing the computer model is provided. In chapter 5, experimental and theoretical results are compared and analyzed. Finally in chapter 6, general observation and recommendations are provided.
Figure 1.1 Front view of a general MBE system
Figure 1.2 Top view of MBE system
CHAPTER 2

LITERATURE REVIEW

2.1 Flow of gases in vacuum systems

Knudsen [21] described the flow of gases in vacuum systems by introducing a
dimensionless number called Knudsen number (Kn). The Knudsen number is defined as
the ratio of mean free path (\( \lambda \)) to the dimensions of the channel through which gas flows.
Mean free path, is frequently encountered in kinetic theory of gases to analyze transport
properties of gases. \( \lambda \) is defined as the average distance traveled by a particle before it
collides with another particle. For a particle with Maxwellian distribution for motion, \( \lambda \) is
given by [22]:

\[
\lambda = \frac{1}{\sqrt{2\pi n\sigma^2}} (cm)
\]  

(2.1)

where \( n \) is the number of particle per unit volume in cm\(^3\), \( \sigma \) is the diameter of the particle
in cm. Combining the equation for ideal gas law and substituting the constants, \( \lambda \) is
obtained as:

\[
\lambda = 7.321 \times 10^{-20} \frac{T}{P\sigma} (cm)
\]  

(2.2)

For a gas flowing through a circular tube of diameter D, the Knudsen number (Kn) is
given by:
When the pressure is high Kn is low, the collisions between the molecules will be more than the collisions with the wall of the tube, and this type of flow is called viscous flow. At low pressures, Kn is high and hence, the collisions among the particles will be lower than the collision with walls of tube. Flow under such conditions is called molecular flow. Between the viscous and molecular flow regimes, there is a region called transitional flow region. In transitional flow, both the particle and wall collision will be comparable and both affect the flow. Knudsen [21] while studying the transition between molecular and viscous flow through a long capillary tube, he plotted the volume flux at centre of the opening of the tube as a function of the mean pressure and reported the existence of a minimum in volume flux called Knudsen minimum. Experiments by many have been done to verify Knudsen's minimum and also theoretical models were developed to explain the phenomenon, for a review on the transitional flow through nozzles and orifices, the reader is referred to Edwards [23].

2.2 Gas-Surface Interactions

Ramsey [24] has reviewed interactions of the molecular beams with the solid surfaces. Most of the laws governing the gas molecule interaction with the surfaces are common to the laws of interaction of photons with surfaces in optics. When a molecule strikes the surface it can rebound from the surface with no loss of momentum and energy or loose so much energy that it gets adsorbed on the surface. In the former case the collisions are elastic and the latter case the collisions are inelastic.
2.2.1 Elastic Collisions

The direction of molecules after an elastic collision has a direct probability relation with the direction of incidence. These molecules can either undergo reflection or diffraction. When the beam of molecules incident on the surface undergo reflection in such a way that the incident beam, the normal to surface of incidence and reflected beam lie in the same plane and the angle of incidence equals angle of reflection then the reflection is said to be specular. For specular reflection to occur, two conditions must be satisfied

a) The height of irregularities (h) on the surface when projected on to the direction of incident beam must be less than the wavelength of the beam. If the glancing angle of incident beam is $\phi_0$ and $\lambda$ De Broglie wavelength of incident molecule then the condition for specular reflection is:

$$h \sin \phi_0 < \lambda$$  \hspace{1cm} (2.4)

b) The average time a molecule spends on the surface must be small.

Estermann and Stern [25] have studied the reflecting properties of helium beam on lithium fluoride (LiF) crystal. Because a crystal surface is smoother than a metal surface, the $h$ in Eq (4) is smaller and hence, the range of $\phi_0$ is more. The above statement was verified by the authors by plotting beam intensity as a function of glancing angle. The range of $\phi_0$ was $0 < \phi_0 < 25^\circ$ for beam temperature of 100°K. They reduced the crystal temperature and observed increase in reflectance power which is in accord with Equation 2.4. This is because $h$, which is the amplitude of oscillations of ions in on the crystal surface, decreases with temperature.
Knauer and Stern [26] have studied the reflecting properties of hydrogen beam on a polished metal surface. They defined the ratio of maximum intensity of the reflected beam to maximum intensity of the incident beam as the reflecting power. They observed a reflecting power of 5% at a glancing angle of $10^{-1}$ at room temperature. They also observed that reflecting power was inversely proportional to beam temperature, which is in accordance with Equation 2.4 because as temperature is reduced $\lambda$ increases.

Diffraction is another important phenomenon observed when molecular beams are reflected from surfaces. Estermann et. al. [27] have done diffraction experiments with helium (He) and hydrogen (H$_2$) molecules impinged on a freshly cleaved LiF crystal. They reported that the results from the diffraction experiments go beyond the electron diffraction methods for they showed that De Broglie relation applied not only to elementary particles but also to atoms and composite molecules. They also checked the mass dependency of wavelength.

2.2.2 Inelastic Collisions

In inelastic collisions, the molecule which strikes the surface can re-evaporate or permanently stick to the surface. In case of re-evaporation, kinematics of the reflected molecule bears no relation to those which prevailed at incidence instead it depends on the kinematics at the last stages of history of the molecule on the surface.

Knudsen [28] studied the angular distribution of re-evaporant mercury molecules after they under went inelastic collisions. In his experiment, he used a spherical glass bulb shown in Figure 2.1. A small portion of upper part (AB) was maintained at room temperature and the remaining part (CD) was cooled. He observed that the layer of mercury deposited on CD was uniform and hence, the angular distribution of re-
evaporated material followed a simple cosine distribution termed as Cosine law of emission. According to cosine law of emission, if \( N \) molecules whose directions lie within solid angle \( d\omega \) strike a surface element \( ds \) for which there is no specular reflection or diffraction, then the number \( dN \) of those re-evaporated from the surface within an element of solid angle \( d\omega \) making an angle \( \theta \) with the normal (shown in Figure 2.2) to the element is given by:

\[
dN = \left( \frac{1}{\pi} N \cos \theta d\omega \right)
\]  (2.5)

Wood [29] has also studied the angular distribution of mercury and confirmed the results of Knudsen’s experiments [28].

Gaede [30] showed that for gas in equilibrium with a surface, the cosine law of emission is a consequence of second law of thermodynamics. In his argument he considered two stationary plates A and B mounted on a rotatable arm and located in an arbitrarily large extent of gas surrounded in an isolating surface as shown in Figure 2.3. The flux of particles incident on either plate in an equilibrium situation is assumed Maxwellian and therefore the incident number flux of particles corresponds to the cosine law. Surface B is assumed to be rough so that each article scatters diffusely according to the cosine law of emission and therefore the collective number flux of all particles leaving this surface must also follow Cosine law. The collective reaction of all particles leaving the arbitrary surface A must also correspond to a cosine scattering, otherwise, the reactions would not balance which will result in the rotation of arm around point M in violation of the second law of thermodynamics. Later Clausing [31] also proved the cosine law of emission through the principle of detailed balance.
Taylor [32] has studied the reflectance power of cesium beam on a NaCl and LiF crystal surfaces. He observed that no specular or diffraction has occurred. He observed cosine law of distribution for reflected molecules as would be expected for molecules adsorbed, equilibrated with the surface and then re-evaporated.

Cosma [33] and Wenaas [34] stressed the importance of distinguishing the 'equilibrium cosine law' and the 'Knudsen law of diffuse scattering'. The Knudsen law of diffuse scattering defines a particular type of scattered particle distribution resulting from a beam of particles incident with any arbitrary speed and direction. The Cosine law of emission, which was previously defined, is same as the Knudsen law of diffuse scattering. The equilibrium cosine law specifies the flux distribution of all particles including reflected, diffracted and desorbed particles from a surface resulting from the equilibrium distribution of incident particles. The Knudsen law of diffuse scattering is usually associated with contaminated or rough surfaces and in no way implies or implied by equilibrium cosine law.

2.3 Angular flux Distribution from Knudsen Cells

Based on a new evaporation technique, Knudsen [35] designed a cell for formation of molecular beams. The Knudsen cell is an isothermal enclosure with a small orifice in it. It contains the source material and its vapor is in thermal equilibrium at a pressure $P_{eq}$. $P_{eq}$ is maintained by having the surface of source material larger than the orifice which causes the Knudsen number to be small and hence, increasing the intermolecular collisions to be higher than wall collisions. The diameter of the orifice should be smaller than the mean free path, $\lambda$ at $P_{eq}$. The wall around the orifice should be vanishingly thin
so that the gas particles passing through the orifice will not be scattered, adsorbed or
desorbed by the orifice wall. Under the above mentioned conditions, the orifice becomes
an evaporating surface and the total number of molecules escaping into vacuum per unit
time is given by:

\[ \Gamma_e = 3.51 \times 10^{22} \frac{P_{eq} A_e}{\sqrt{MT}} \quad \text{(molecules/sec)} \]

where \( A_e \) is area of the orifice, \( M \) is molecular weight in gms, \( P_{eq} \) is pressure in Knudsen
cell in Torrs, \( T \) is temperature in Kelvin. The molecules which effuse into the vacuum do
not undergo collisions between themselves as the pressure is so low that the Knudsen
number is high. Knudsen also predicted the angular distribution of flux to be cosine
(shown in Figure 2.4) which is called as the Cosine law of effusion. Using the Cosine law
of effusion and Equation 2.6 it can be shown that the flux for geometry shown in Figure 2.5
is given by [15]:

\[ I_A = \frac{\Gamma_e}{\pi r_A^2} \]

At A:

\[ I_B = I_A \frac{r_A^2}{r_B} \cos \theta \cos(\theta + \phi) \]

where \( r_A \) is radius of element around point A and \( r_B \) is radius of element around point
B.

Clausing [36] has given theoretical formulation for determining the angular
distribution from the Knudsen cells with circular orifice of finite thickness. For his
calculation, he employed two gas chambers connected by a cylindrical tube of length,
\( l_c \) and diameter, \( d_o \). The first gas chamber is an isothermal enclosure with gas molecules
at pressure $P_{eq}$. The molecules leave the first chamber under molecular flow conditions and enter the second chamber where pressure is close to zero (UHV). The molecules entering the tube undergo wall collisions but not intermolecular collisions. The total number of molecules which arrive in the second chamber have two components. The first component consists of molecules which arrive directly from the evaporant surface formed at the entrance of the cylindrical tube and is given by:

$$d\Gamma_p = \left(3.51 \times 10^{22} \frac{P_{eq} A_e}{\sqrt{MT}}\right) \cos \theta d\omega \left[1 - \frac{2}{\pi} \left(\sin^{-1} p + p\sqrt{1-p^2}\right)\right] \text{(molecules/sec)}$$  \hspace{1cm} (2.9)

where $A_e$ is the area of the orifice given by:

$$A_e = \frac{\pi d_o^2}{4}$$  \hspace{1cm} (2.10)

$M$ is molecular weight of effusing species, $T$ is the temperature of first chamber, $d\omega$ is the solid angle subtended at the centre of entrance to cylindrical tube by an area $ds$ at an angle $\theta$ to tube axis, $p$ is given by

$$p = \frac{l_o}{d_o} \tan \theta, \text{for } \theta \leq \tan^{-1}\left(\frac{d_o}{l_o}\right)$$  \hspace{1cm} (2.11)

The second component is the flux reflected from the walls of the orifice and is given by:

$$d\Gamma_w = \left(3.51 \times 10^{22} \frac{P_{eq} A_e}{\sqrt{MT}}\right) \cos \theta d\omega B$$  \hspace{1cm} (2.12)

where $B$ is a coefficient which depends on $\theta$ and is given by

$$B\left(\theta \leq \frac{d_o}{l_o}\right) = \frac{2\alpha}{\pi} \left(\sin^{-1} p + p\sqrt{1-p^2}\right) + \frac{4(1-2\alpha)}{3\pi} \left(\frac{1-(1-p^2)^{3/2}}{p}\right)$$  \hspace{1cm} (2.13)
\[
B\left( \theta \geq \frac{d_o}{l_o} \right) = \alpha + \frac{4(1-2\alpha)}{3\pi p}
\]  
(2.14)

where
\[
\alpha = \frac{\sqrt{l_o^2 + d_o^2 - l_o}}{d_o + d_o/\sqrt{l_o^2 + d_o^2}}
\]  
(2.15)

Hence, the total flux, which is the sum of the two flux components given by Equations 2.9 and 2.12, for \( \theta \leq \tan^{-1}\left(\frac{d_o}{l_o}\right) \) is given by:
\[
d\Gamma = d\Gamma_\theta + d\Gamma_w
\]  
(2.16)

For \( \theta \geq \tan^{-1}\left(\frac{d_o}{l_o}\right) \) the molecules coming directly from orifice entrance are blocked by the walls of the tube and hence the only flux is \( d\Gamma_w \) which is given by Equation 2.12. The net effect on the flux distribution due to finite thickness is that the distribution is narrower than that expected by the cosine law of effusion as shown in Figure 2.6.

Clausing [37] derived a formula for the total flux of molecules coming out of an orifice of finite thickness. He modified the common expressions for molecular flow by the introduction of kinetic variables and gave the formula:
\[
K = W S\nu
\]  
(2.17)

where \( K \), is the number of molecules per second coming out of the orifice, \( W \) is a dimensionless quantity and represents the transmission probability (also known as Clausing's coefficient), \( S \) is the cross sectional area of the orifice, and \( \nu \) is the number of molecules per unit area per unit second which strike the inner walls of the cell. Value of \( W \) varies with of length to diameter ratio, \( (l_o/d_o) \), of the orifice and these values were
calculated by Clausing and reported in [37]. Based on Clausing’s formulation the
Equation 2.6) is modified as:

\[ \Gamma_0 = 3.51 \times 10^{22} \frac{P_{eq} A W}{\sqrt{M T}} \text{(molecules/sec)} \]  

(2.18)

It is to be noted that Equation (18) does not have any effect on the normalized angular
distribution of flux, but does affect the absolute number for flux.

Motzfeld [38] derived the formula for the total flux of molecules at the exit of the
orifice to include the pressure variation in the cell. Equation 2.6 was derived assuming
that the cell has a small orifice and that the pressure inside \( (P_{eq}) \) is same everywhere in
the cell. Due to non ideal orifice having considerable radius, the pressure will be different
in different planes parallel to the source material. The expression for the total flux under
conditions mentioned above and derived by Motzfeld is given by:

\[ \Gamma_e = 3.51 \times 10^{22} \frac{P_{eq} A W}{M_z \sqrt{M T}} \text{(molecules/sec)} \]  

(2.19)

where

\[ M_z = 1 + \frac{A_e W_e}{A_c} \left( \frac{1}{\alpha} + \frac{1}{W_c} - 2 \right) \]  

(2.20)

\( P_{eq} \) is the pressure inside the cell if the cell were ideal, \( W_e \) is Clausing’s coefficient for the
orifice, \( A_e \) is area of the orifice, \( M \) is the molecular weight of the evaporating species, \( T \) is
the temperature, \( A_c \) is area of the cell, \( \alpha \) is the evaporating coefficient for the material
used in the cell and \( W_c \) is the Clausing’s coefficient for the body of cell. Equation 2.20
suggests that the pressure non uniformity affects the net flux, but not the angular
distribution of the flux.
2.3.1 Surface Diffusion and Specular Reflection

Winterbottom [39] has shown inadequacies of Clausing’s work and proposed a new model including surface diffusion effects on the angular distribution. Clausing’s work was based on diffuse reflection model for vapor solid interaction. In diffuse reflection model the impinging molecule will reflect at the point of collision according to the cosine law of emission. Previous results [40] did not agree with diffuse reflection model, so Winterbottom proposed a new model called Coupled Vapor Transport model. In the new model, the adsorbed molecule will be characterized by mobility and a time of stay on the surface that is related to the binding between the molecular species and the orifice surface. In the new model, flux distribution is not only dependent on the geometrical factors but also on the temperature and material of the orifice. The model employs diffusion distance given by:

\[ \bar{x} = \sqrt{\frac{2}{E}} \]  

(2.21)

where

\[ E = \frac{\varepsilon}{D_s} \]  

(2.22)

\( \varepsilon \) is evaporation probability per unit time, \( D_s \) is surface diffusivity. In the limiting condition of \( E \to \infty, \bar{x} \to 0 \) the model reduces to the Clausing’s model. According to the model flux distribution will be less focused along the axis of cell than the distribution predicted by Clausing. The author also reported that surface diffusion influence the near ideal orifice and not the longer orifices. The results obtained with the new model are in qualitative agreement with the experimental results.
Dunham and Hirth [41] have extended Winterbottom’s [39] calculation for cylindrical channel to conical channel. The conical channels are used to reduce the focusing effect of the cylindrical channel. The authors obtained quantitative flux considering not only geometrical factors, but also surface diffusion effects on the channel walls. Their calculation of total flux is comprised of three components: fluxes from the cell interior, the channel wall and the cell lid. The flux from the cell interior comprises of molecules from the evaporant surface formed at the entrance orifice. The molecules from the evaporant cell obey the Cosine law of effusion. The re-evaporation of molecules adsorbed on channel wall contributes to the second component. The second component is a function of geometry and surface diffusion. For a given geometry, different effusate cell materials have different surface diffusivities and desorption energies. The third component is a result of some adsorbed molecules on channel wall diffusing on to the cell lid before they are lost to the surroundings. The three components were obtained by solving integro-differential equations formulated based on Winterbottom’s model [39]. One of the important parameters obtained from their calculation is transmission coefficient defined as the ratio of actual molecules that effuse at the end of channel to the number of molecules that enter the channel. From their calculations they reported that the surface diffusion does not affect the general shape of the flux distribution but strongly affects the transmission coefficient. They also reported that the geometry has significant effect on the flux distribution and the transmission coefficient. They concluded that the conical channels have higher transmission coefficient than the cylindrical channels and less focusing effect, even if the surface diffusion effects are considered.
2.3.2 Angular distribution of flux dependence on evaporating species

A series of experiments with different gas species like Cadmium and Cesium Chloride effusing from channels made with different materials like copper, pyrex and nickel were performed. The complete details of the experiments are given in their papers [42-45]. Here, only the important design considerations and results are discussed. The important design consideration is the use of a double oven effusion cell. The first oven was maintained at a temperature $T_B$ to set the vapor pressure of gas and second oven was set at temperature $T_F$ to adjust mean free path of the gas species. In their experiments in molecular flow regime, they observed that:

(a) The transmission coefficient $\Psi$ and probability of effusion along axis of cell $P(0)$ showed dependence on the difference between the two ovens $\Delta T = T_F - T_B$. For short cylindrical channel $\left( \frac{l_0}{d_o} < 1 \right)$, $\Psi$ is independent of $\Delta T$, $P(0) \propto \Delta T$ and for long cylindrical channel $\left( \frac{l_0}{d_o} > 1 \right)$, $\Psi \propto \Delta T$, $P(0) \propto \frac{1}{\Delta T}$.

(b) As the length of the orifice increased, the velocity distribution of molecules along axis of orifice became increasingly distorted from a Maxwellian distribution with too many high speed molecules along the axis of the cell.

(c) The angular distribution of flux deviated from that predicted by the Clausing's model.

The authors discussed the possible reasons for the above observations. They ruled out the gas phase collisions in the channel and surface diffusion effects on the channel wall as these two effects cannot explain distortion in the velocity distribution. They concluded that a possible explanation could be the departure of emission of molecules from the channel walls, from the Cosine law of emission. The departure from the cosine law was
explained as due to the specular reflection of high speed molecules coming at low or moderate angles at the wall.

Ward et. al. [46] have conducted experiments with small Knudsen cells at high temperature. For the pressure and temperature used in their experiments, there were few gas phase collisions in the cell and hence, the kinetic theory could not explain the behavior of individual gas atoms and also the Cosine law of effusion cannot be used. The effusing beam was made up almost entirely of molecules that came directly from some surface inside the cell. Their Knudsen cell consisted of a knife edge orifice, the walls of the cell were coated with tantulum or graphite and the effusate materials like plutonium or gold were located in a cup at the centre of the bottom of the cell. The cup materials were Y2O3, MgO and ThO2. The main aim of these experiments was to test if cosine law had any dependence on type of material used for the cell and effusate. With plutonium, they observed deviations from the Cosine law as plutonium is highly reactive with cup and cell wall materials. With gold in tantalum cells, they observed deviations from the cosine law as gold reacted with tantalum. They observed that for gold in graphite, the flux distribution followed the Cosine law, as gold is not reactive with graphite. They observed that the sample shape can have effect on the flux distribution at angles close to the axis of the cells. Flat samples produced a double hump and spherical sample produced a centre hump in the flux distribution. They formed a model based on Monte Carlo technique to study the geometric parameters, physical and chemical losses which effect the flux distribution [47]. In their model, the direction of emitted particle from the effusate surface follows the cosine law of emission and wall reflections were assumed diffuse. They assigned different loss probabilities to different parts of the cell, cup wall,
cell wall and lid wall. All their experimental results were in good agreement with that of the Monte Carlo model. This proves the validity of surface emission concept for small cells at high temperature.

Ward et.al used Monte Carlo techniques to obtain flux distribution from Knudsen cells with cylindrical [48] and conical channels [49]. They assumed that the Knudsen cells are large enough to create gas phase collisions in vapor inside the cell that at the entrance of the channel, a uniform flux source, effusing molecules under the Cosine law of effusion was formed. They included specular reflection and surface diffusion effects in their simulations. Specular reflection was modeled as probability $\psi$ given by:

$$\psi = c \exp\left(\frac{-\alpha}{a}\right)$$

where $c$ and $a$ are arbitrary constants and $\alpha$ is the incident angle. The surface diffusion was modeled by considering a normalized distribution for diffusion length. The results for cylindrical channel agreed qualitatively with Wang et.al.[42]. Their results for surface diffusion showed excellent agreement with Winterbottom [39] results and their plots were smoother than Winterbottom because they chose a normalized distribution function for diffusion length instead of fixed diffusion lengths. Due to specular reflection the flux distribution seem to fall off faster than the case with diffuse reflection. In case of surface diffusion the flux distribution was not effected for long channels. Their results for conical channels agreed well with Dunham and Hirth [41]. They observed that for conical channels, AD due to specular reflection and surface diffusion fell off faster than that with diffuse reflection and surface diffusion.

Carson et. al. [50] reported deviations from the Cosine law of emission. They evaporated an alloy under molecular flow conditions in a bell jar vacuum system.
According to the Cosine law the film deposited on the walls of the spherical shell should be uniform but they observed that at high evaporation rates, the evaporant was found to be concentrated in a direction normal to the melt surface. They did not give any reason for the observed phenomenon.

Grimley et. al. [51-54] obtained AD of species from polymeric vapor systems such as KCl, AgCl, CuCl and Bi. They observed that all the flux distributions deviated from the Clausing’s theory and the flux distribution of various species varied from one another. For ideal orifice, the detectable deviations were small but as $I_s/d_s$ increased, deviations from Clausing’s theory became more pronounced, with the data showing positive deviations at lower angles and negative deviations at higher angles. They also showed that experimental results for same vapor species could be different if different channel material is used i.e. BN and Ta. They also reported that the flux distribution for dimer specie is more focused than that of monomer specie [55].

Later Winterbottom [56] proposed modification in his old model [39] to predict the difference in monomer and dimer flux distribution. He suggested that flux distribution can be predicted if it is assumed that the species are chemisorbed and characterized by appropriate diffusion length in the adsorbed state. For the dimer, a heterogenous surface reaction involving the disassociative adsorption of the dimer and a monomer association for the reverse reaction to form a desorbable dimer species, accounts for the observed flux distribution. His results showed qualitative agreement with experimental results of Grimley et.al [55].
2.3.3 Knudsen cell Design

Shen [57] published a work for an industrial Knudsen cell with a large single opening, 0.84 cm in diameter and another cell with 240 small openings, each opening is 0.0787 cm in diameter and 0.78 cm long. He calculated the angular distribution of small openings by considering 32 locations and calculating angular distribution from each location using Clausing's formula and finally summing up the individual distributions to obtain final distribution. When he applied corrections due to distance variations between different source points and substrate, he obtained good agreement between his calculated and experimental results. Thus, he proved that Clausing's theory and the superposition principle can be applied for calculating flux distribution for multichannel ovens. His calculation for large opening did not match experimental results. He reasoned that there are many possible forms of interaction between different sections of the orifice in a dynamic evaporating situation.

Cho and Cheng [58] reported for the first time the rotation of substrate in MBE systems to obtain excellent thickness uniformity of wafers. Even though flux arriving at substrate is non-uniform, the rotation causes a averaging of the non uniform and hence, gives uniform thickness of epilayer. They performed three experiments to evaluate uniformity of the layers. In the first experiment they used interference measurement techniques to determine the uniformity of growth rates and found that variation on 5 cm wafer rotated at 2 rpm was only 1%. The uniformity of chemical composition measured using photoluminescence showed that Al$_{0.3}$Ga$_{0.7}$As alloy composition is uniform to 0.004 AlAs mole fraction, over 4 cm wafer. In the third experiment the distribution of carrier concentration and the pinch off voltage of a thin n-type layer grown on a semi-insulating
substrate was done to determine the uniformity of impurity concentration and yield of the wafer. They found that variation in pinch off voltage was only 1.4% over a 4 cm wafer.

Dobrowolsi et. al. [59] reported an improved Quartz Crystal Monitor setup to obtain the flux distribution. Their setup consisted of 2 crystals, one of which was fixed above the source and the other swung on an arc centered on the source. The plotted output becomes a ratio of flux from a moving crystal to flux from a fixed crystal, which provided a normalized output and eliminated errors due to change in the ratio of evaporation during one scan period. With their apparatus, they obtained flux distribution under various conditions for source shown in Figure 2.7.

They found that all the angular distributions could be represented by analytical expressions of the type given by:

\[
I(\theta) = \cos^x \theta + A \sin^2 B \theta
\]  

(2.24)

Where \(x\), \(A\) and \(B\) are constants determined from the experimental results by a root mean square fitting procedure. Measurements of flux in different planes cutting through the axis of source were measured. They found the curves from various planes coincide and hence, proving that the flux is symmetrical. They found that angular distribution for cell with orifice is more cosine than that of an open cell. They found that angular distribution of cell with 45° flare showed significant positive deviations in flux profile at higher angles compared to the cell with no flare. They found that as rate of evaporation increases, the deposition at lower angles is greatly enhanced which is suggested to be due to higher pressure and vapor scattered region that forms above source mouth. They reported different flux distributions for source species like Cryolite and Zinc Sulphide.
ZnS was found to be more directional than Cryolite. They found that the level of material in the cell had no effect on the flux distribution.

Maki. et.al.[60] have reported that conventional conical cells exhibit significant flux transients upon shutter opening due to cooling of melt surface. They designed a new cell which utilizes a deep pyrolytic boron nitride (PBN) insert to maintain beam uniformity. The temperature of the melt deep in the furnace is less sensitive to changes in radiative shielding provided by the cell shutters. Deep cells with no insert exhibit poor uniformity due to change in the projected melt area at large angles from cell axis. For cells with insert, the unobstructed melt area is constant even for large angles from cell axis and hence the uniformity is improved. Their results from the electron mobility experiments indicated that the purity of epitaxial layer is not affected. Beam equivalent pressure measurements indicated that flux transients were less for new cell with insert compared to the flux transients of the conventional cell.

2.3.4 Computer simulation methods

Curless [61] used computer simulations for obtaining the flux distribution for conical cells. He assumed the source material to be at a single temperature and each point on surface of source puts out flux according to the cosine law of emission. The rate of evaporation at a point on the wall of the cell is taken to be equal to the incident flux on the wall at that point, unless that point is defined as being wetted by the source material. In the case where the point on the wall is wetted by the source material the rate of evaporation is assumed to be equal to that of the source material. The effect of surface diffusion and also any interaction between molecules were ignored. The program allows user to enter data related to geometry of the cell, geometry of the source material,
orientation of the cell with the substrate, wetted portion of cell wall and areal evaporation rate for the source material. The general formula used to calculate flux ($dF$) from a point $P'$ to a point $P$ on substrate is given by:

$$
dF = \frac{E(\hat{n}' \cdot \vec{V})(-\vec{V} \cdot \hat{n})da'}{\pi(\vec{V} \cdot \vec{V})}
$$

(2.25)

where $E$ is areal rate ($#/cm^2\cdot sec$) at which molecules leave at $P'$, $\hat{n}'$ is the unit normal to surface at $P'$, $\vec{V}$ is the vector from $P'$ to $P$, $\hat{n}$ is the unit normal to the substrate at $P$ and $da'$ is the area of region containing $P'$. For calculating flux on wall portion which is not wetted, he noted that as the cell and source material are symmetric about the axis of the cell, it is only necessary to calculate flux on any straight line along the wall. The flux at any point of the un-wetted wall had three components; the first is from the bottom of the cell, second from the wetted portion of the wall and the third from other portion of un-wetted wall. The first two components were calculated by Equation 2.25 and last component is calculated iteratively, i.e., first the flux on all un-wetted portions is set to be the flux from bottom ($F_B$) plus flux from wetted portion ($F_W$). The flux to that point from un-wetted portion is calculated iteratively till the change of flux is less than 1%. He applied the model to the growth of the GaAs without rotation of substrate with reactor geometry similar to that of Varian GEN II system. The model showed that gallium flux varied by 30% and Gallium to Arsenic ratio varied by a factor of two over 4 cm$^2$. These results were in reasonable agreement with experimental data. He also suggested that neglecting flux contribution from the cell wall decreases the accuracy of the model, but gives qualitatively the same picture.

Wasilewski et. al. [62] have used numerical methods based on Curless [61] work to obtain the flux distribution for conical cells. They modeled two cells used in V80H MBE.
system. The first cell (CL1) had a tapering angle of $1.3^\circ$ and the second cell (CL2) has a tapering angle of $8^\circ$. They measured thickness of material deposited in two stages: in the first stage a relative thickness variation across the wafer using a scanning reflectance system was obtained and in the second stage, absolute thickness profile was constructed using reflectance spectroscopy. For their theoretical model, they assumed cosine law on all evaporating surfaces. They neglected surface diffusion based on the argument that the diffusion length is smaller than element size used for the grid. One major difference between this work and Curless work [61] is that Curless assumed that the melt surface is always perpendicular to wafer even though the cell is tilted but in the present work, the exact position and orientation are calculated taking into account the cell shape, its spatial orientation and the un-tilted melt distance. From their observation of cells used in actual experiments, they noted the formation of melt droplets at the opening of the cell. To take this effect into account, they used different re-evaporation coefficient for that part of the cell, where droplets were found.

For flux distribution calculations they represented the layer of droplets by an annular ring. From their calculations they observed that for same amount of material used, CL1 produced thicker layer than CL2 at the expense of worse layer uniformity. They proved using their calculation that neglecting flux from walls will change the shape of angular distribution as opposed to Curless’s observation [61]. They observed that even though the separate components of flux are affected by the angle of the melt, the net profile is not affected. Their experimental results had a maximum deviation of 0.5% and 1% from the calculated values for CL1 and CL2 respectively. The diameter of droplets had significant effect on the flux distribution. The most crucial parameter, which affected the flux
distribution, was the melt level. They also obtained thickness for rotated substrate. They observed that as the cell is tilted so that the intersection of axis of cell with wafer moves towards the centre of the wafer, the uniformity became better. They observed that when the angle between the normal to wafer and cell axis is changed (cell axis always intersects the centre of wafer) the uniformity changes and there is an optimum angle for which the uniformity is best i.e. 45° for their system.

Wasilewski et. al. [63] performed simulations for the cell design suggested by Maki et. al. [60]. They later [64] improved the design and implemented it in their experimental work. The cell consists of a main cell to hold the material charge and a flux shaping conical insert. They modeled the new cell assuming an equivalent melt at the bottom of the insert. They found that the tilt of melt had no effect on the flux distribution and hence consider that melt surface was always perpendicular to the axis of the insert. They observed that the melt level in the new cell did not effect the angular distribution. The new cell gave an added advantage that flux could be reshaped by choosing an appropriate insert. The layer uniformity of the new cell was better than the simple conical cell. The difference between Maki et. al. design [60], and the present design is that Maki et. al. [60] used a cell, where the axis of the main cell and insert coincided whereas in Wasilewski et. al. design the axes were separated by an angle. The present design resulted better uniformity than Maki et. al. [60] design.

Aers and Wasilewski [65] studied the effect of changing the cell to substrate distance. They investigated the cell design shown in Figure 2.8. They observed that the uniformity increased in the following order, cylindrical cell, conical cell, cylindrical cell with orifice, and cylindrical cell with conical tilted insert. As the substrate to cell distance increased,
the cylindrical cells with and without orifice showed slow rate of uniformity improvement. The conical cell showed increased rate of improvement in layer uniformity as the cell was pulled back from substrate. The cylindrical cell with conical tilted insert showed a great increase in uniformity over a specific distance, but beyond the specific distance, there was practically no improvement.
Figure 2.1 Experimental Setup used by Knudsen to demonstrate Cosine Law of Emission

Figure 2.2 Solid angles in which molecules strike and re-emit
Figure 2.3 Configuration used by Gaede for explaining Cosine law of emission

Figure 2.4 Flux distribution from an ideal Knudsen cell.
Figure 2.5 Geometry of ideal Knudsen cell and substrate.

Figure 2.6 Diagram showing the flux distribution from the Knudsen cell with finite thickness, according to Clausing's calculations.
Figure 2.7 Various cell designs studied by Dobrowolsi et al. [40]. (a) Cylindrical cell (b) Cylindrical cell with orifice (c) Cylinder with funnel on top (d) Cylinder with funnel and a flare.

Figure 2.8 Various cell designs studied by Aers and Wasilewski [46]. (a) Cylindrical cell (b) Cylindrical cell with orifice (c) Conical cell (d) Cylindrical cell with tilted conical insert.
CHAPTER 3

MATHEMATICAL FORMULATION AND NUMERICAL METHODS

3.1 Introduction

The number of molecules passing per unit time per unit area is termed as flux. The distribution of flux in all possible directions is called angular or spatial distribution of flux. Angular distribution of flux from the Knudsen cell is an important factor as it decides the uniformity of thickness of epitaxial layers grown in the Molecular Beam Epitaxy (MBE) technique. Angular distribution of flux depends on the temperature, pressure and geometry of the cells used in MBE. The temperature and pressure decide the flow regime in which the cell is operating. In most of the applications, the cell is operated in the molecular flow regime and hence all further discussion will be limited to this regime. For complete description of the regimes the reader is referred to Section 2.1. The physics behind the emission process in different cells are discussed in following paragraphs.

3.2 Types of emission

The process of emission of molecules from the melt surfaces in the Knudsen cells fall into two categories, they are Langmuir and Knudsen modes of emission.
3.2.1 Langmuir mode of emission

In Langmuir mode of emission, any solid or liquid surface has a specific ability to emit and cannot exceed a certain maximum emission rate at a given temperature even if the supply of heat is unlimited. Theoretical maximum rate of emission are obtained only if as many evaporant molecules leave the surface as would be required to exert the equilibrium pressure on the same surface and none of them returning to the surface. Langmuir mode of emission is also called as free emission.

3.2.2 Knudsen mode of emission

In Langmuir mode of emission, the condition that molecules leaving the condensed phase of melt surface do not return is not always satisfied. For instance, the molecules leaving the condensed phase could be reflected by the vapor as shown in Figure 3.1. To avoid these discrepancies Knudsen [35] suggested an alternative technique known as Knudsen emission. In Knudsen emission technique, emission occurs as effusion from a Knudsen cell which is an isothermal enclosure with a small orifice. The evaporating surface within the enclosure is large compared with the orifice and maintains the equilibrium pressure inside. The diameter of the orifice must be less than one tenth of the mean free path of the gas molecules at the equilibrium pressure and the wall around the orifice must be vanishingly thin so that gas particles leaving the enclosure are not scattered by the orifice wall. Under these conditions the orifice, constitutes an evaporating surface with the inability to reflect molecules back into enclosure. The mathematical formulation describing the direction of emission is given in following paragraphs.
3.3 Cosine law of effusion

The interaction between the surface of the condensed phase and an individual atom about to emit determines the direction in which the particle will be emitted. Since the distribution of kinetic energies among molecules is well known for gaseous state, the spatial distribution of particles can be derived for the effusion of gases from an ideal Knudsen cell and extend the analysis to free emission [1].

An ideal Knudsen cell with orifice area \( dA \) is shown in Figure 3.2. The cell is assumed to contain \( N \) molecules whose population is maintained constant by the presence of condensed phase. The molecules are assumed to have a Maxwellian speed distribution and these molecules collide with the walls of cell reflecting back without causing a net change in the total speed distribution. Molecules moving toward the orifice will escape retaining the direction and speed prior to escape. Under such a condition, the spatial distribution of flux in effusing beam can be determined by the distribution of molecular speeds inside the effusion cell.

The flux is represented by number of molecules per unit area per unit time escaping into a small solid angle \( d\omega \). The solid angle is the 3-D analog of the usual definition of angle. Mathematically the solid angle is defined as the ratio of the area of the object which the solid angle encloses, to the square of the radius of the sphere of which the object is a part. For the case shown in Figure 3.2, the area of the object which the solid angle encloses is \( dA \), the centre of the sphere coincides with centre of the orifice and the radius of the sphere is the distance, \( r \) between object and the orifice. Hence the expression for \( d\omega \) is given by:
The spatial distribution is represented by an expression which relates flux in all directions from the normal to the orifice and the expression can be derived by the following procedure.

Let \( \phi(c^2) \) represent the speed distribution of all molecules in the container, then the number of molecules \( dN_c \) having speeds within \( c \) and \( c+dc \) is given by:

\[
dN_c = N\phi(c^2)dc
\]

Since the directions of the molecules inside the Knudsen cell are randomly distributed over the total solid angle \( 4\pi \), the fraction of molecules which enter the solid angle \( d\omega \) is given by:

\[
dN_\omega = \frac{d\omega}{4\pi}
\]

The molecules with speed \( c \) which escape out of the orifice within a time \( dt \) and an angle \( \varphi \), are confined in the slanted cylinder shown in the Figure 3.2. The area of the orifice is \( dA_e \). If \( V \) represents the total volume of the cell, then the fraction of molecules which escape in direction \( \varphi \) is given by:

\[
dN_\nu = \frac{cdt\cos\varphi dA_e}{V}
\]

Combining equations 3.1 to 3.3, the number of molecules per unit time with speed \( c \) which escape into solid angle \( d\omega \) in a direction \( \varphi \) is given by:

\[
d^t_{c,\omega,\varphi,\nu}(\varphi) = \frac{N\phi(c^2)c\cos\varphi dc d\omega dA_e dt}{4\pi V}
\]
with '4' in the superscript on 'c' in LHS of above equation representing that it is a fourth order derivative. Integrating the above equation over all speeds Equation 3.4 modifies to:

$$d^3N_{\omega,\tau} (\varphi) = \frac{N \cos \varphi d\omega dA}{4\pi V} \int_0^\infty \phi(c^2) c \, dc$$

where $c$ is the mean speed and recognizing that

$$\Gamma = \frac{1}{4 V} N c \quad (cm^2 s^{-1})$$

where $\Gamma$ is total number of molecules effusing from orifice per unit time per unit area in all directions also known as areal rate of emission. Rearranging terms in equation 3.5 we get

$$dF_e(\varphi) = \frac{d^2}{dt \, dA_e} (dN_{\omega,\tau} (\varphi)) = \Gamma \cos \varphi \frac{d\omega}{\pi} \quad (cm^2 s^{-1})$$

where $dF_e$ is the number of molecules per unit time per unit area of the orifice, escaping into solid angle $d\omega$ in the direction of angle $\varphi$ to normal of the surface of effusion. $dF_e(\varphi)$ represents angular or spatial distribution of flux and is known as the Cosine law of effusion. The factor $\cos \varphi$ in Equation 3.7 represents the directionality of effusing molecules and is termed as distribution function, $F(\varphi)$.

Since the flux effusing from the orifice into any direction is known, the flux received by any element in space can be calculated. The total number of molecules passing through $dA_e$ per unit time is given by multiplying the flux evaporating from the orifice in the direction $\varphi$, with the area of the orifice. The flux received by the area $dA_e$ is obtained
by dividing the number of molecules passing through it by its area. Substituting the expression for solid angle from Equation 3.0 in Equation 3.7, the expression for flux received is given by:

\[
dF_r = \frac{\Gamma \cos \varphi \, dA_e}{\pi r^2} \quad (cm^{-2}s^{-1})
\]

Equation 3.8

Note that the incident beam of flux is normal to the area \(dA_e\). If the area is inclined at angle other than \(90^0\) to the direction of incident beam, then a component of the normal flux is received by the area. For example, for the area \(dA_e'\) which is inclined at \(\theta^0\) from the normal to incident beam, as shown in Figure 3.2, the flux received is given by the expression:

\[
dF_r = \frac{\Gamma \cos \varphi \cos \theta \, dA_e}{\pi r^2} \quad (cm^{-2}s^{-1})
\]

Equation 3.9

The general observations that can be made from Equation 3.9 are, the flux received by an element is,

1) Directly proportional to the areal rate of emission (\(\Gamma\)) from the source element.
2) Directly proportional to the angle (\(\cos \varphi\)) between the normal to the source element and the line joining the centers of source and receiving elements.
3) Directly proportional to the angle (\(\cos \theta\)) between the normal to the receiving element and the line joining the centers of source and receiving elements.
4) Directly proportional to the area (\(dA_e\)) of the source element.
5) Inversely proportional to the square of the distance (\(r\)) between source and receiving elements.
6) The term \(1/\pi\) is the constant of proportionality.
3.4 Cosine law of evaporation

The Cosine law of effusion can be extended to liquid and solid surfaces under free emission. The argument of support is that the distribution of energies and directions of molecules emerging from a surface cannot differ from an equilibrated vapor without violating the second law of thermodynamics. The surface area of emission should be small and should not be subject to any entropy constraints and in practice these conditions are met for free emission of simple solids and liquids with monatomic vapor and therefore the Cosine law can be extended to most of the evaporant materials. For detailed description of constraints on the use of Cosine law and experimental proof the reader is referred to Hirth and Pound [66]. Since the process of free emission involves the process of evaporation, the Cosine law describing the process is named as Cosine law of evaporation.

3.5 Angular distribution of flux from practical cells

The cells used in MBE are designed to carry large amounts of source material as this helps in larger run time. Hence the cell design varies from an ideal cell. The shape of the cells used can be categorized into cylindrical and conical. The cells are further classified as with and without orifice. The physics of emission is quite different for cells with the orifice and cells without the orifice (open cells).

3.5.1 Non-Equilibrium cells

In the cells without the orifice the surface area of the source material is equal to or smaller than the area of the opening. In cylindrical cells the surface area of the source material and opening is equal. In conical cells the surface area of the source material is
smaller than the opening. In these cells the condensed phase and vapor of source material are not in thermodynamical equilibrium with one another hence these cells are also called as non-equilibrium cells. Even though the emission process is free emission, Cosine law of evaporation cannot be directly applied as the surface area is large. One way of analyzing these cells is to use the method proposed by Shen [57]. In Shen’s method the large surface is divided into smaller elements and Cosine law of evaporation (Equation 3.9) is applied to each element. The final angular distribution is obtained by superimposing the flux from all the elements.

3.5.2 Equilibrium cells

In cells with orifice, whatever be the shape of the cell the surface area of source material is always greater than the area of the orifice. In ideal cells the area of the orifice is much smaller than melt surface but in practical cells this not the case. In practical cells the orifice area is made larger to get larger emission rates. In these cells the condensed phase and vapor of source material are in thermodynamic equilibrium with one another, hence these cells are called equilibrium cells. The physics of emission is similar to Knudsen emission (effusion), in which the vapor at entrance of orifice becomes the source of flux. In previous section it was shown that for an ideal Knudsen cell with small orifice the molecules effuse according to Cosine law of effusion.

In practical cells the orifice area being large and cell not being maintained at perfect isothermal condition, the Cosine law of effusion with its cosine distribution function \( F(\phi) = \cos(\phi) \) for flux cannot be directly applied. The distribution function is modified to take into all non idealities and is given by:
where \( N \) is a positive real number and \( \phi \) is angle from normal to surface of orifice. The function suggests that as \( N \) increases the molecules are increasingly focused towards the normal to surface of orifice.

### 3.5.2.1 Modified Cosine law of effusion

With the modified distribution function the Equation 3.9 for flux received will also be modified. The modification involves two changes and they are,

1) The flux received is directly proportional to the power \( N \) of the angle \( \cos^N \phi \) between the normal to the source element and the line joining the centers of source and receiving elements.

2) The constant of proportionality \( 1/\pi \) is modified to a new constant \( C \).

All the remaining observations will remain the same. The modified equation for flux received is of the form:

\[
dF_r = C \Gamma \frac{\cos^N \phi \cos \theta dA_s}{r^2} \quad (cm^{-2}s^{-1})
\]

The new constant of proportionality \( C \) is derived as follows. The orifice represents a source surface with no ability to reflect back molecules into the Knudsen cell and hence molecules are emitted into a hemisphere shown in Figure 3.3. The centre of the hemisphere is the centre of the orifice. The number of molecules per unit time crossing the area \( dA \) is given by \( dN_r = dF_r dA \). From Figure 3.3 the area \( dA = r^2 \sin \phi \, d\phi \, d\phi \), substituting these terms in Equation 3.11, the equation becomes:

\[
dN_r = C \Gamma dA_s \cos^N \phi \cos \theta \sin \phi \, d\phi \, d\phi
\]
Since the element $dA_\epsilon$ is normal to the incident beam, substituting $\theta = 0^\circ$ in Equation 3.12 results in:

$$dN_\epsilon = CT \, dA_\epsilon \cos^N \phi \sin \phi \, d\phi \, d\phi$$

Integrating Equation 3.13 over the whole hemisphere will yield the total number of molecules crossing the hemisphere per unit time which is equal to the total number of molecules per unit time emitted from the orifice surface. The total number of molecules emitted is given by the product of areal rate of emission ($\Gamma$) and area of the orifice ($dA_\epsilon$).

Hence equating the terms results in:

$$\int_0^{2\pi} \int_0^{\pi/2} C \Gamma \, dA_\epsilon \cos^N \phi \sin \phi \, d\phi \, d\phi = \Gamma \, dA_\epsilon$$

which gives

$$C = \frac{N + 1}{2\pi}$$

Substituting Equation 3.14 in Equation 3.11 results in:

$$dF_\epsilon = \frac{N + 1}{2\pi} \Gamma \cos^N \phi \cos \theta dA_\epsilon$$

Equation 3.15 represents the modified Cosine law of effusion. It can be noted that by substituting $N=1$ in the above equation, the equation is exactly similar to Equation 3.9. The physical significance of $N$ is to represent the focusing effect of molecular beams from practical cells. As $N$ increases, the probability of molecules effusing in a direction normal to the orifice increases.
3.6 Numerical Methods

In practical cells the source is not a small element but is large enough to be considered as a surface. The flux received at a point in space is calculated by integrating Equation 3.15 over the surface of the source and the expression is given by:

$$F_r = \int \int dF_r$$  \hspace{1cm} 3.16

Since analytical integration of Equation 3.16 is impossible due to complicated nature of the source surface, the source surface is divided into small elements or grid elements. Integration is approximated by a summation of flux from each grid element and is given by:

$$F_r = \sum_{i=1}^{n} dF_{ri} = \sum_{i=1}^{n} \frac{N+1}{2\pi} \frac{\cos^\psi \phi_{ri} \cos \theta_{ri} dA_{ei}}{r_i^2}$$  \hspace{1cm} 3.17

where \(n\) represents the number of grid elements into which the source surface is divided.

For numerical computation, the term, \(\cos \phi_{ri}, \cos \theta_{ri}\) and \(r_i\) in Equation 3.16 have to be determined. The source and destination elements are shown in Figure 3.4. \(P_{si}(x_{si1}, y_{si1}, z_{si1}), P_{si2}(x_{si21}, y_{si21}, z_{si21}), P_{si3}(x_{si31}, y_{si31}, z_{si31})\) and \(P_{si4}(x_{si41}, y_{si41}, z_{si41})\) are corner points of source element. \(P_{di}(x_{di1}, y_{di1}, z_{di1}), P_{di2}(x_{di21}, y_{di21}, z_{di21}), P_{di3}(x_{di31}, y_{di31}, z_{di31})\) and \(P_{di4}(x_{di41}, y_{di41}, z_{di41})\) are corner points of destination grid element. The point \(P_{si}(x_{si1}, y_{si1}, z_{si1})\) and \(P_{di}(x_{di1}, y_{di1}, z_{di1})\) are the centroid of the source and destination grid elements respectively and their co-ordinates are given by:

\[
\begin{align*}
x_{si} &= \frac{x_{si1} + x_{si21} + x_{si31} + x_{si41}}{4}, \quad y_{si} = \frac{y_{si1} + y_{si21} + y_{si31} + y_{si41}}{4}, \quad z_{si} = \frac{z_{si1} + z_{si21} + z_{si31} + z_{si41}}{4} \\
x_{di} &= \frac{x_{di1} + x_{di21} + x_{di31} + x_{di41}}{4}, \quad y_{di} = \frac{y_{di1} + y_{di21} + y_{di31} + y_{di41}}{4}, \quad z_{di} = \frac{z_{di1} + z_{di21} + z_{di31} + z_{di41}}{4}
\end{align*}
\]
The unit normal to source grid element is $\vec{n}'$ and is given by the cross product of vectors forming the sides of the source grid element.

$$n'_i = \frac{P_{sli}P_{s2i} \times P_{sli}P_{s4i}}{|P_{sli}P_{s2i}||P_{sli}P_{s4i}|}$$

where $\overline{P_{sli}P_{s2i}}$ is vector joining points $P_{sli}$ and $P_{s2i}$, and $\overline{P_{sli}P_{s4i}}$ is vector joining points $P_{sli}$ and $P_{s4i}$. The expressions for the vectors are given by:

$$\overline{P_{sli}P_{s2i}} = (x_{s2i} - x_{sli})\hat{i} + (y_{s2i} - y_{sli})\hat{j} + (z_{s2i} - z_{sli})\hat{k}$$

$$\overline{P_{sli}P_{s4i}} = (x_{s4i} - x_{sli})\hat{i} + (y_{s4i} - y_{sli})\hat{j} + (z_{s4i} - z_{sli})\hat{k}$$

The vector joining $P_{s}$ and $P_{d}$ is $\vec{r}_{i}$ and is given by:

$$\vec{r}_{i} = (x_{d} - x_{sli})\hat{i} + (y_{d} - y_{sli})\hat{j} + (z_{d} - z_{sli})\hat{k}$$

cos $\phi_{i}$ is calculated from dot product of normal to source grid element and vector $\vec{r}_{i}$ and the expression is given by:

$$\cos \phi_{i} = \frac{\vec{n}'_{si} \cdot \vec{r}_{i}}{|\vec{n}'_{si}| |\vec{r}_{i}|} \quad 3.18$$

Following in the steps similar to the ones for obtaining cos $\phi_{i}$ the expression for cos $\theta_{i}$ is given by dot product of normal to source grid element and vector $\vec{r}_{i}$ and the expression is obtained as:

$$\cos \theta_{i} = \frac{\vec{n}'_{si} \cdot -\vec{r}_{i}}{|\vec{n}'_{si}| |-\vec{r}_{i}|} \quad 3.19$$

where $\vec{n}'_{d}$ is the unit normal vector to the destination area around $P_{d}$ and is given by:
\[ \vec{n}'_d = \frac{\vec{P}_{d1} \times \vec{P}_{d4}}{| \vec{P}_{d1} \times \vec{P}_{d4} |} \]

where \( \vec{P}_{d1} \) is vector joining points \( P_{d1} \) and \( P_{d2} \) and \( \vec{P}_{d4} \) is vector joining points \( P_{d1} \) and \( P_{d4} \). The expressions for the vectors are given by:

\[
\vec{P}_{d1} \times \vec{P}_{d4} = (x_{d2} - x_{d1}) \hat{i} + (y_{d2} - y_{d1}) \hat{j} + (z_{d2} - z_{d1}) \hat{k}
\]

\[
\vec{P}_{d1} \times \vec{P}_{d4} = (x_{d4} - x_{d1}) \hat{i} + (y_{d4} - y_{d1}) \hat{j} + (z_{d4} - z_{d1}) \hat{k}
\]

It is noted that \( r_i^2 \) is the square of the absolute value of vector \( \vec{r}_i \) and is given by:

\[ r_i^2 = | \vec{r}_i |^2 \]

The area \( dA_{ei} \) of source grid element is given by the magnitude of the cross product of the vectors which form the sides of the grid element as shown in Figure 3.5 and the expression is:

\[ dA_{ei} = | \vec{P}_{si} \times \vec{P}_{s4i} | \]

Equations 3.17-3.22 provide a way to numerically obtain the flux at point outside the cell. The flux will be computed at all points on the required surface to give the flux distribution on that surface.
Figure 3.1 Condensed Phase and Vapor of Source Material in Thermodynamical Equilibrium showing reflection of molecules at the interface.

Figure 3.2 Knudsen cell with molecules effusing from orifice of area $dA_e$ into the solid angle $d\omega$ at an angle $\varphi$ from normal to the cell orifice. Element $dA_r$ at a distance $r$ is receiving flux from the element $dA_e$. 

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Figure 3.3 An element $dA$, on surface of the orifice effusing molecules in to the hemisphere.

Figure 3.4 Vectorial representation of source and destination grid element
4.1 Sumo Cell Description

The cell under consideration is a 10,000g Sumo cell which belongs to the class of SUMO cells patented by VEECO. Unique properties of SUMO cells are listed below [67].

1) The cells unique design reduces the thermal load on the system which in-turn reduces the release of impurities from chamber walls. The reduction of impurities leads to purer epitaxial films.

2) The defects found in epitaxial films are reported to be low due to the orifice design and the heat shielding cap. The orifice is efficiently heated to reduce any condensation of material.

3) SUMO cells have substantially greater charge capacity over corresponding standard cells.

4) Shutter related transients are reduced because the melt surface is recessed within the cell and the front heat shielding serves as a thermal baffle between melt and shutter.

5) SUMO cells reduce the depletion effect by providing a constant melt surface.
6) SUMO cells come with dual filament feature, in which the orifice temperature is maintained at a different temperature than that of the main body of the cell. The orifice is maintained at a higher temperature for Gallium (Ga), Indium (In), etc. to avoid condensation of material. The orifice is maintained at a lower temperature to avoid creeping of materials like aluminum out of the cell.

The geometry and dimensions of the 10,000g SUMO cell are shown in Figure 4.1. For the purpose of analysis, the cell is divided into two portions, the main body and the orifice as shown in Figure 4.1. The main body and the orifice are connected through a neck region which will also be referred to as opening of the cell or entrance to the orifice section.

For obtaining angular distribution of flux from the cell, two models were formulated based on two possible types of emission. In the first model (Model I), it was assumed that free evaporation occurs from the melt surface. An ideal Knudsen cell is expected to have an opening of very small diameter compared to the body of the cell for Knudsen effusion to occur. But in the cell under consideration, the inner orifice diameter (1.5 inches) is only three times smaller than the main body of the cell (4 inches) and hence there is a possibility that the cell was acting as a non-equilibrium cell and molecules undergo free evaporation.

In the second model (Model II), it is assumed that the Knudsen effusion occurs from the flux source formed at the opening of the cell. The cosine law of effusion with the distribution function \( F(\phi) = \cos \phi \) cannot be applied to the cell under consideration as the inner orifice diameter is quite large and also the cell is not isothermal as all SUMO cells are provided with dual filament feature in which the orifice is maintained at different temperature from the main body of the cell. Details of these two models are presented.
and discussed in separate sections in this chapter. Results of these models will be discussed in the next chapter.

4.2 Model I

In Model I, the cell is treated as a non-equilibrium cell hence analysis will be done based on the method described in section 3.5.1. The whole melt area is treated as a surface composed of a number of evaporating sources emitting molecules according to the Cosine law of evaporation. A portion of the flux from the melt area will arrive at the walls of the cell and will be re-emitted according to cosine law of evaporation. Specular reflection and surface diffusion effects are neglected assuming that they are not significant for the cell under consideration.

Flux reaching any point outside the cell has two components. One component is the flux coming directly from the melt surface known as primary flux and the second component is the flux coming from exposed portions of inner wall surface of the cell, known as secondary flux. The setup of the cell and platen are shown in Figure 4.2. $x_{pla}$ is the distance between cell and platen, $\theta_{ali}$ is tilt of the cell with respect to platen, and $r_{pla}$ is the radius of the platen. $m_{lev}$ is the liquid level in the cell, $\hat{n}_{pla}$ and $\hat{n}_{melt}$ are the unit normal to platen and melt, respectively. The model is also capable of giving flux distribution for platen which is rotated about the center. In the following sections, the generation of points on the platen at which flux values are calculated, and grid generation on the surface of the cell and the melt surface are discussed.
4.2.1 Generation of points on platen

The platen is that portion of the MBE system which holds the wafers on which epitaxial layers are grown. In MBE systems used for research purposes the platen usually holds one wafer, but in commercial systems, the platen is designed to hold multiple wafers. For example, the GEN2000 a commercial system is used to hold seven 6 inch wafers. The platen in commercial system is rotated azimuthally to reduce flux nonuniformities.

In this model, the user is allowed to choose \( r_{\text{pla}} \). To account for rotation of the platen, points are generated on concentric circles on the platen. The flux calculated on a circle will be averaged to obtain flux on that circle. The process is repeated for each circle of varying radius to obtain the rotated platen flux distribution. For mathematical treatment, the setup of the platen, cell and co-ordinate axis are shown in Figure 4.3. For generating the points, the platen is initially considered to lie on the yz plane as shown in Figure 4.3.

The pattern of points generated is shown in Figure 4.4. The user is allowed to choose the number of points \( m_{p1} \) on the innermost circle and also the number of circles \( n_r \) on the whole platen. With these information provided, the radius of the \( i^{\text{th}} \) circle \( (r_i) \) and number of points on that circle \( (m_{pi}) \) will be given by:

\[
\begin{align*}
  r_i &= \frac{ir_{\text{pla}}}{n_r} \quad \text{(4.1)} \\
  m_{pi} &= i m_{p1} \quad \text{(4.2)}
\end{align*}
\]

Knowing \( r_i \) and \( m_{pi} \), the actual co-ordinates of points on the \( i^{\text{th}} \) circle can be calculated. To calculate the co-ordinates of \( j^{\text{th}} \) point on \( i^{\text{th}} \) circle as in Figure 4.5, note that the angle subtended by a circular arc joining any two adjacent points is same and is given by:
\[
\Delta \phi = \frac{360^\circ}{m_{pi}} \tag{4.3}
\]

Hence, the angle \((\phi_j)\) subtended by the line joining the center of the platen and \(j^{th}\) point to the positive y-axis is given by:

\[
\phi_j = j \Delta \phi \tag{4.4}
\]

Hence, \(y\) and \(z\) co-ordinates are given by:

\[
y_j = r_j \cos \phi_j \tag{4.5}
\]
\[
z_j = r_j \sin \phi_j \tag{4.6}
\]

Note that the \(x\) coordinate is same for all points as the platen is lying on the \(yz\) plane and is given by \(x_j=x_{pln}\). Knowing the co-ordinates of all the points on the platen on the \(yz\) plane, the co-ordinates for these points on platen tilted at angle \(\theta_{tilt}\) to the \(x\)-axis can be obtained by applying rotational transformation as shown below.

\[
\begin{bmatrix}
x_{i,j} \\
y_{i,j} \\
z_{i,j}
\end{bmatrix} =
\begin{bmatrix}
\cos \theta_{tilt} & -\sin \theta_{tilt} & 0 \\
\sin \theta_{tilt} & \cos \theta_{tilt} & 0 \\
0 & 0 & 1
\end{bmatrix}
\begin{bmatrix}
x_j \\
y_j \\
z_j
\end{bmatrix}
\]

4.2.2 Grid on the surface of cell

The walls of the cell contribute the secondary flux. To calculate this flux, the cell wall has to be divided into small elements. Division into elements is done by laying a grid on the wall, and these elements can be of any shape. But in the present model, trapezoidal grid elements are used as they are easy to generate and utilize in numerical computation.

The cell under investigation can be viewed as a pack of circles of varying radii with their centers lying on the \(x\)-axis as shown in Figure 4.6. The cell has a circular symmetry around the \(x\)-axis. In order to determine the radii of the circles, the 2-d profile of cell
lying in the xz plane is sampled at different locations. The locations of the points are
chosen at where curve changes shape as shown in Figure 4.7. The sampled x-coordinate’s
and corresponding radii are stored in arrays \(xsam\) and \(rsam\).

The points sampled provide a general 2-D profile of the cell, to generate closely
packed circles the sampled points will be interpolated and radii at the desired \(x\) will be
obtained. The number of circles \((grid_v)\) to be packed is provided by the user from which
the spacing between any two adjacent circles \((dv)\) can be calculated by the equation given by:

\[
dv = \frac{xsam(last) - xsam(first)}{grid_v}
\]  

Since \(dv\) is known, the x-coordinate after interpolation \((xint)\) is given by \(xint_i = i \cdot dv\), where
\(i\) ranges from 0 to \(grid_v\). Given the x-coordinates, the radius at these locations is
obtained by interpolation between the sampled \(rsam\) values. For \(xint_i\), which lies between
\(xsam_j\) and \(xsam_{j+1}\), \(rint_i\) is obtained by linear interpolation given by the equation:

\[
rint_i = \frac{rsam_{j+1} - rint_j}{xsam_{j+1} - xsam_j}
\]

In the above equation \(rint_i\) is the only unknown. Small values of \(grid_v\) leads to highly
non uniform surface for the cell and at the same time, very high \(grid_v\) leads to increase
in computation time.

The circles in the cell can be viewed as vertical sections of the grid. In order to form
the whole grid, horizontal sections should also be generated. Due to the symmetry of the
cell, the horizontal grid can be generated in any quadrant and then, mapped into other
quadrants. In the present analysis, the grid will be generated in quadrant I and then
mapped into quadrants II, III, and IV. The user is allowed to choose the number of
horizontal sections (grid_h) in the 1st quadrant.

The horizontal grid is generated by rotating the 2-D profile shown in Figure 4.7
"grid_h" number of times around the x-axis. The 2-D coordinates x_int and r_int in three
dimensions will become x_{oi}=x_{int_i}, y_{oi}=0 and z_{oi}=r_{int_i}, these coordinates form the plane
xz_o as shown in Figure 4.8. After one rotation the co-ordinates on xz_o will move to
xz_1. The angular increment (ΔΨ) through which the plane xz_o is rotated is given by:

$$\Delta\psi = \frac{90^\circ}{\text{grid}_h}$$

4.9

The new coordinates of the point after rotating (x_{0i}, y_{0i}, z_{0i}) through angular increment
ΔΨ as shown in Figure 4.9 are given by: x_{il} = x_{0i}, y_{il} = z_{0i} \sin(\Delta\psi), and
z_{il} = z_{0i} \cos(\Delta\psi). In general after the jth rotation, the new coordinates are given by x_{ji}=
x_{0i}, y_{ji} = z_{0i} \sin(j\Delta\psi), and z_{ji} = z_{0i} \cos(j\Delta\psi).

For coding purposes, the cell coordinates in first quadrant are stored in matrix format
as shown below:

$$X_i = \begin{bmatrix}
x_{i1} & \cdots & x_{ij} & \cdots & x_{i(grid_h+1)} \\
\vdots & \ddots & \vdots & \cdots & \vdots \\
x_{i1} & \cdots & x_{ij} & \cdots & x_{i(grid_h+1)} \\
\vdots & \ddots & \vdots & \cdots & \vdots \\
x_{(grid_v+1)i} & \cdots & x_{(grid_v+1)j} & \cdots & x_{(grid_v+1)(grid_h+1)} \\
\end{bmatrix}$$

$$Y_i = \begin{bmatrix}
y_{i1} & \cdots & y_{ij} & \cdots & y_{i(grid_h+1)} \\
\vdots & \ddots & \vdots & \cdots & \vdots \\
y_{i1} & \cdots & y_{ij} & \cdots & y_{i(grid_h+1)} \\
\vdots & \ddots & \vdots & \cdots & \vdots \\
y_{(grid_v+1)i} & \cdots & y_{(grid_v+1)j} & \cdots & y_{(grid_v+1)(grid_h+1)} \\
\end{bmatrix}$$
The complete grid on cell surface after mapping the co-ordinates to remaining quadrants is shown in Figure 4.10. The coordinates, thus formed on the surface of the cell, can be grouped to form grid elements. The number of grid elements that can be formed with grid_v vertical sections and grid_h horizontal sections is (grid_v)(grid_h). Since the grid elements are trapezoidal, the coordinates have to be grouped in four to form a grid element. For example, to form the grid element shown in Figure 4.11, the coordinates to be grouped are \( P_1(x_1, y_1, z_1), P_2(x_2, y_2, z_2), P_3(x_3, y_3, z_3), P_4(x_4, y_4, z_4) \). In general, for grid element ‘k’ the points are given by \( P_1(x_{i,j}, y_{i,j}, z_{i,j}), P_2(x_{i+1,j}, y_{i+1,j}, z_{i+1,j}), P_3(x_{i,j+1}, y_{i,j+1}, z_{i,j+1}), P_4(x_{i+1,j+1}, y_{i+1,j+1}, z_{i+1,j+1}) \).

In order to calculate the flux from the grid elements we need the centroids, normals and the areas of the grid elements and these can be obtained by the process described in section 3.6. If \( Xcen, Ycen \) and \( Zcen \) represent the matrices which carry the x, y and z coordinates of the centroids in the first quadrant, then the matrices containing the centroids of the entire cell are given by:

\[
Xcen = \begin{bmatrix}
Xcen_1 & Xcen_2 & Xcen_3 & Xcen_4
\end{bmatrix}_{(grid_v)(grid_h) \times 4}
\]

\[
Ycen = \begin{bmatrix}
Ycen_1 & Ycen_2 & Ycen_3 & Ycen_4
\end{bmatrix}_{(grid_v)(grid_h) \times 4}
\]

\[
Zcen = \begin{bmatrix}
Zcen_1 & Zcen_2 & Zcen_3 & Zcen_4
\end{bmatrix}_{(grid_v)(grid_h) \times 4}
\]

If \( Xunc, Yunc \) and \( Zunc \) represent the matrices containing the unit normals to grid elements on the cell in the first quadrant, then the matrices containing the unit normals to entire cell are given by:

\[
Z = \begin{bmatrix}
z_{11} & \ldots & z_{1j} & \ldots & z_{1(grid_h+1)} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
z_{i1} & \ldots & z_{ij} & \ldots & z_{i(grid_h+1)} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
z_{(grid_v+1)1} & \ldots & z_{(grid_v+1)j} & \ldots & z_{(grid_v+1)(grid_h+1)} \\
\end{bmatrix}
\]
\[
X_{\text{unc}} = \begin{bmatrix} X_{\text{unc}_1} & X_{\text{unc}_1} & X_{\text{unc}_1} & X_{\text{unc}_1} \end{bmatrix}_{(\text{grid}_{-v}) \times \text{grid}_{-h}} \\
Y_{\text{unc}} = \begin{bmatrix} Y_{\text{unc}_1} & Y_{\text{unc}_1} & -Y_{\text{unc}_1} & -Y_{\text{unc}_1} \end{bmatrix}_{(\text{grid}_{-v}) \times \text{grid}_{-h}} \\
Z_{\text{unc}} = \begin{bmatrix} Z_{\text{unc}_1} & -Z_{\text{unc}_1} & -Z_{\text{unc}_1} & Z_{\text{unc}_1} \end{bmatrix}_{(\text{grid}_{-v}) \times \text{grid}_{-h}}
\]

If \( Ac_i \) is the matrix containing the area of grid elements in the first quadrant, then the matrix containing the area of the grid elements on the entire surface of the cell is given by:

\[
Ac = [Ac_i \ Ac_i \ Ac_i \ Ac_i]
\]

The unit normals and centroids, thus formed, are shown in Figure 4.12.

4.2.3 Grid on the melt surface

The process of evaporation from the melt surface is free evaporation. The cosine law which governs the directionality of evaporating molecules cannot be directly applied to the entire surface as the surface is not a plane. Instead, the surface is divided into smaller elements which can be approximated as a plane and then the law is applied to each element. The division into smaller elements is done by laying a grid and the process is discussed below.

The parameters which describe the melt in the cell are melt level \((mlev)\) and angle of tilt of the melt surface with respect to the cell axis. The melt level is the distance of the center of the melt surface from the orifice opening measured along the cell axis and should be provided by the user. Since the melt surface is always parallel to platen, the normal to platen and melt surface will be parallel to one another but in opposite directions. Thus, the angle between surface and cell axis will be \(90^\circ - \theta_{\text{tilt}}\) as shown in Figure 4.13. In order to lay a grid on the melt surface, the coordinates describing the boundary of the surface should be known. These coordinates of intersection can be obtained by solving the equation of the plane in which the melt surface lies, and the equation of the surface of the cell.
If $\mathbf{P}$ is the normal from the origin to the plane and $(l, m, n)$ are the direction cosines of the normal, then the equation of the plane is given by:

$$lx + my + nz = \lvert \mathbf{P} \rvert \quad (-\infty \leq x \leq \infty, -\infty \leq y \leq \infty, -\infty \leq z \leq \infty) \quad 4.10$$

The plane under consideration is shown in Figure 4.13. Note that the plane is parallel to the y-axis. The directions cosines are given by $l = \cos \theta_{\text{tilt}}$, $m = 0$, $n = -\sin \theta_{\text{tilt}}$. $\lvert \mathbf{P} \rvert$, is the perpendicular distance of plane from the origin and given by $\lvert \mathbf{P} \rvert = (mlev) \cos \theta_{\text{tilt}}$.

Substituting these parameters in Equation 4.10, the equation of the plane can be obtained.

$$x - mlev = \tan \theta_{\text{tilt}} z \quad 4.11$$

The above equation has to be solved with the surface of the cell to get the boundary coordinates. In the process of laying grid on the cell, the cell surface was described as pack of circles and is treated the same here. Hence, the surface of the cell is described by:

$$y^2 + z^2 = r^2(x) \quad (0 \leq x \leq 15.557) \quad 4.12$$

The values of $x$ and $r$ for the cell were obtained by interpolation process described under Equation 4.7 and 4.8, and are stored in arrays $x_{\text{int}}$ and $r_{\text{int}}$. The $y$ and $z$ coordinates of melt boundary are calculated at $x_{\text{int}}$ using Equations 4.11 and 4.12 and are given by:

$$z_i = \frac{x_{\text{int},i} - mlev}{\tan \theta_{\text{tilt}}} \quad 4.13$$

$$y_i = \pm \sqrt{r_{\text{int},i}^2 - z_i^2} \quad 4.14$$

In Equations 4.13 and 4.14, only real solutions represent the melt boundary. The boundary is symmetric about x-axis which is also observed in the solutions for $y_i$ which
take equal positive and negative values. The solutions, thus, obtained are stored in arrays \(xbound, ybound\) and \(zbound\).

For a given \(\theta_{ult}\), not all values of \(mlev\) are valid. As shown in Figure 4.14, the melt will overflow from the cell for certain values of \(\theta_{ult}\) and \(mlev\). This condition usually occurs for low \(mlev\) and high \(\theta_{ult}\). To avoid such a condition, the equations 4.13 and 4.14 are solved for the position of limiting circle shown in Figure 4.14. If any solution for \(y_i\) and \(z_i\) exist, the user will be asked for higher \(mlev\) for \(\theta_{ult}\) provided by him and the new boundary is determined.

As the coordinates of the boundary are known, a user specific grid can be laid within the boundary. The vertical spacing along the x-axis is taken to be the spacing between circles of the cell (grid_v), and the user will specify the horizontal spacing along the y-axis (\(m_.h\)). The grid elements are rectangular and hence, four corner points are needed to define any grid element. The order of the corner points \(P1, P2, P3\) and \(P4\) are shown in Figure 4.15. The coordinates of the corner points of the first grid element are \(P11(\text{xbound}_1, \text{ybound}_1, \text{zbound}_1)\), \(P21(\text{xbound}_2, \text{ybound}_1, \text{zbound}_2)\), \(P31(\text{xbound}_2, \text{ybound}_1-m_.h, \text{zbound}_2)\), \(P41(\text{xbound}_1, \text{ybound}_1-m_.h, \text{zbound}_1)\). The coordinates for adjacent grid element are \(P12=P11, \ P22=P21, \ P32(\text{xbound}_2, \text{ybound}_1-2(m_.h), \text{zbound}_2), \ P42(\text{xbound}_1, \text{ybound}_1-2(m_.h), \text{zbound}_1)\). The y-coordinate is, thus, decremented till the other end of the boundary is touched. The process is repeated for all values in the arrays \((\text{xbound}, \text{ybound}, \text{zbound})\) to get the grid on entire melt surface.

Once, the grid elements are formed, the centroids, normals and area can be calculated by procedure outlined in section 3.6. Note that the normal to the melt surface and the area
of any grid element is same everywhere on the surface and need to be computed once for any grid element.

4.2.4 Flux on walls of the cell

The cell walls contribute considerable flux to the platen. Before calculating this flux, it is necessary to calculate the flux on the wall itself. The flux received by the walls from the melt surface need not be same for all the grid elements on wall. In the following paragraphs, the process of calculating flux on walls for a given melt surface orientation is discussed.

4.2.4.1 Flux on walls directly from melt surface

The cell and melt surface are symmetrical about the x-axis and hence, the exposed wall of the cell is also symmetrical. Therefore, the flux can be computed for half of the cell wall as shown in Figure 4.16 and then, mapped on to the other half. Flux will be calculated at the centroids of the grid elements on the wall. Note that not all grids can see the whole of the melt surface. The cell is divided into four sections as shown in Figure 4.17 and the division is based upon whether the grid elements can receive any direct flux from melt surface. The portion of the melt surface from which the grid element can receive flux is said to be visible else the portion is invisible.

The section I of the four divisions is the orifice portion of the cell. The elements on the wall of the orifice do not receive direct flux from the entire portion of the melt surface as shown for point P₁ in Figure 4.17. In order to determine the portion of melt surface visible to a grid element, the equation of straight lines joining P₁ and all centroids of grid elements on melt surface are formed and checked if they pass through the limiting circle formed at the neck of the cell. Let us consider the following example, let coordinates of
$P_1 (x_1, y_1, z_1)$ and coordinates of any point $P_2$ which is the centroid on the melt surface be $(x_2, y_2, z_2)$ as shown in Figure 4.18. The equation of the straight line joining $P_1$ and $P_2$ is given by:

$$\frac{x - x_1}{x_2 - x_1} = \frac{y - y_1}{y_2 - y_1} = \frac{z - z_1}{z_2 - z_1}$$

4.15

This line has to be checked if it passes through the limiting circle at neck shown in Figure 4.18. This can be done by calculating the y, z coordinates of point of intersection of straight line given by Equation 4.15 and plane of limiting circle given by equation:

$$y^2 + z^2 = r_{\text{limit}}^2$$

4.16

where $r_{\text{limit}}$ is the radius of the limiting circle and is known. If $P_3$ is the point of intersection then the coordinates are given by solving Equation 4.15 and 4.16 and the equations are:

$$x_3 = x_{\text{limit}}, y_3 = \frac{x_{\text{limit}} - x_1}{x_2 - x_1} (y_2 - y_1) + y_1, z_3 = \frac{x_{\text{limit}} - x_1}{x_2 - x_1} (z_2 - z_1) + z_1$$

Where $x_{\text{limit}}$ is the location of the limiting circle and is known. The condition to be satisfied for $P_2$ to be visible to $P_1$ is:

$$y_3^2 + z_3^2 < r_{\text{limit}}^2$$

For determining the portion seen by $P_1$, the process is repeated for all the centroids of grid element on the melt surface.

In section II of the four divisions, all the points on wall belong to the main body and can see the entire melt surface. In section III, the points belong to the main body of the cell and some lie inside the melt and some outside. In order to check if the point lies outside the melt surface, the z-coordinate is compared (Figure 4.19). To determine $P_2$
location, since the coordinates on the boundary of melt surface which lies in Section III is known, \( z_{\text{bound}} \) is known for every \( x_2 \). If \( z_2 > z_{\text{bound}} \), then the point lies outside, otherwise the point lies on or inside the melt surface. In section IV, all points lie inside the melt surface and hence the flux will not be calculated for grid elements on this portion of the wall.

After checking the points on half of the cell for their location, flux is obtained according to the cosine law of evaporation for melt described in section 3.6 and the formula is given by

\[
F_{W - M - P_j} = \sum_{i=1}^{n} \frac{\Gamma \cos \varphi_{ni} \cos \theta_{di} dA_i}{\pi r_i^2}
\]

where \( n \) is the number of grid elements on the melt surface point \( P_j \) on wall can see, \( \Gamma \) is the areal rate of emission for melt surface and is assumed to be \( 1/\text{in}^2\text{s}^{-1} \), for all elements on the melt. \( \theta_{di} \) is angle between normal to the melt surface and the line joining the centroid \( P_i \) of the grid element on the melt and \( P_j \). \( \theta_{di} \) is angle between the normal to the grid element on the wall and line joining \( P_i \) and \( P_j \). \( r_i \) is the distance between \( P_i \) and \( P_j \) and \( dA_i \) is the area of the grid element on the melt.

4.2.4.2 Multiple Wall Collisions

The flux received by the wall elements from the melt surface will be redistributed among the wall elements through the process of multiple wall collisions. Any grid element on the wall is exposed to the rest of wall grid elements and hence receives flux from them and in turn emits flux to them. This process continues till steady state condition is achieved and the flux distribution on the whole wall does not change. The steps involved for simulating multiple wall collision is described in following paragraph.
The flux on each of the grid element on wall from melt is calculated by the process described in section 4.2.4.1. The total flux received by the entire wall from the melt remains constant under steady state conditions. The total flux on wall is calculated by summing the flux received by each wall element and is stored in variable $F_{W_M}$. If the grid element at which flux is to be calculated is in the II or III sections (exposed main body) as shown in the Figure 4.17, then the element can see all the grid elements in II and III sections and few elements in section I (orifice).

If the element is in section I of the cell, then it can see all the elements on the wall of section I and few elements on sections II and III of the cell. The visible portions whether on section I or section II and III are determined by the process described in section 4.2.4.1. The flux from visible portions of the wall at the wall element, whose centroid is $P_j$, is calculated by the formula:

$$F_{W_W_P_j} = \sum_{i=1}^{n} \frac{(F_{W_M_P_i}) \cos \varphi_i \cos \theta_{di} dA_i}{\pi r_i^2}$$

4.18

where $n$ is the number of grid elements on the wall, point $P_j$ can see. $F_{W_M_P_i}$ is the areal rate of emission or flux for the wall grid element whose centroid is $P_i$ and was calculated in section 4.2.4.1. $\varphi_i$ is angle between normal to wall element around $P_i$ and line joining $P_i$ and $P_j$. $\theta_{di}$ is angle between normal to wall element around $P_j$ and line joining $P_i$ and $P_j$, $r_i$ is the distance between $P_i$ and $P_j$ and $dA_i$ is the area of grid element around $P_i$.

The flux is thus calculated for all the grid elements and represents the flux after single wall collision. The total flux on the entire wall ($F_{W_W}$) should be equal to steady state total flux from melt $F_{W_M}$. Hence, the flux at each wall element after wall collision is normalized by the expression:
\[ F_\sim W \sim P_j = (F_\sim W \sim W \sim P_j) \frac{F_\sim W \sim M}{F_\sim W \sim W} \]

4.19

The process is repeated again to get flux distribution on wall after second wall collision but this time the areal rate of emission for elements on wall will be flux calculated by Equation 4.19. The process is repeated till the change in value of flux at any grid element on wall is less than 1%. Thus the flux on the walls is calculated.

4.2.5 Flux on Platen

As discussed previously in section 4.2, the flux has two components, primary flux from the melt surface and the secondary flux from the walls of the cell. The two components are calculated separately at the various points generated on the platen. The two components are added up at each point to get the total flux distribution on the platen. The points on platen see varying portions of the cell wall and the melt surface.

For example, consider a point \( P_i(x_i,y_i,z_i) \) on the platen and \( P_j(x_j,y_j,z_j) \) centroid of the \( j \)th grid element on the melt. In order to check for visibility the following procedure is adopted. Firstly, the equation of the straight line joining \( P_i \) and \( P_j \) is formed as shown below:

\[
\frac{x-x_i}{x_j-x_i} = \frac{y-y_i}{y_j-y_i} = \frac{z-z_i}{z_j-z_i}
\]

4.20

Since the \( x \)-coordinates, \( x_{lim1} \) and \( x_{lim2} \) of limiting circles 1 and 2 shown in Figure 4.20, are known, the same \( x \)-coordinates will be used for intersecting points \( P_1 \) and \( P_2 \). The \( y \) and \( z \) coordinates of \( P_1 \) and \( P_2 \) will be given by substitution of \( x \)-coordinates in Equation 4.18. The equations are:

\[
x_1 = x_{lim1}, \quad y_1 = \frac{x_{lim1} - x_i}{x_j - x_i} (y_j - y_i) + y_j, \quad z_1 = \frac{x_{lim1} - x_i}{x_j - x_i} (z_j - z_i) + z_i
\]

79
\[ x_2 = x_{\text{lim1}} - x_i, y_2 = \frac{x_{\text{lim1}} - x_i}{x_j - x_i}(y_j - y_i) + y_i, z_2 = \frac{x_{\text{lim1}} - x_i}{x_j - x_i}(z_j - z_i) + z_i \]

Since the radius \( r_{\text{lim1}} \) and \( r_{\text{lim2}} \) of limiting circle 1 and 2 are known, the conditions for visibility are \( y_1^2 + z_1^2 < r_{\text{lim1}}^2 \) and \( y_2^2 + z_2^2 < r_{\text{lim2}}^2 \). Both the conditions must be simultaneously satisfied for visibility. The process is repeated for all the grid elements on the melt surface and exposed cell. Note that only condition \( y_1^2 + z_1^2 < r_{\text{lim1}}^2 \) has to be satisfied for the grid elements on the orifice section.

The flux from the visible portion of melt surface to point \( P_i \) on platen is given by:

\[ F_{\text{melt}} P_i = \sum_{j=1}^{n_m} \frac{\Gamma \cos \varphi_{ij} \cos \theta_{ij} dA_j}{\pi r_j^2} \quad 4.21 \]

where \( n_m \) is the number of grid elements on the melt surface point \( P_j \) on the platen can see. \( \Gamma \) is the areal rate of emission for the melt surface and is assumed to be 1(in\(^2\)s\(^{-1}\)) for all elements on the melt. \( \varphi_{ij} \) is the angle between the normal to the melt surface and the line joining \( P_j \) and \( P_i \). \( \theta_{ij} \) is the angle between the normal to the platen and the line joining \( P_i \) and \( P_j \). \( r_i \) is the distance between \( P_i \) and \( P_j \) and \( dA_j \) is the area of grid element on the melt.

The flux from the visible portion of the exposed cell wall to the point \( P_i \) on the platen is given by:

\[ F_{\text{wall}} P_i = \sum_{j=1}^{n_w} \frac{(F_{\text{wall}} P_j) \cos \varphi_{ij} \cos \theta_{ij} dA_{wj}}{\pi r_j^2} \quad 4.22 \]

Where \( n_w \) is the number of grid elements on the wall, point \( P_i \) on platen can see. \( F_{\text{wall}} P_j \) is the flux emitting from the centroid of the \( j \)th grid element on the wall, \( P_j \). \( \varphi_{ij} \) is the angle between the normal to the grid element on wall and line joining \( P_j \) and \( P_i \). \( \theta_{ij} \) is
angle between normal to the platen and line joining $P_i$ and $P_j$. $r_i$ is the distance between $P_i$ and $P_j$, and $dA_{ij}$ is the area of the grid element on the wall.

The total flux at point $P_i$ on the platen is given by:

$$F_{-P_i} = F_{-Pr_i} + F_{-Sec_Pj}$$  \[4.23\]

The total flux calculated using Equation 4.23 at all points on the platen called un-rotated flux, which represents the flux distribution on a stationary platen. On a rotated platen, the flux on any circle on the platen surface with its center coinciding with center of the platen will be constant and the flux at every point on a circle will be the same. As discussed in section 4.2.1, it was shown that the points are generated on a concentric circle. The flux on any circle on the rotated platen is called the rotated flux and is given by averaging the un-rotated flux at all points on the circle and the equation is given by:

$$F_{-R_r_i} = \sum_{i=1}^{n} \frac{F_{-P_i}}{n}$$  \[4.24\]

where $r_i$ is the radius of the circle on which rotated flux is calculated, $n$ is the number of points on the circle, and $F_{-P_i}$ is the total flux at point $P_i$ on the circle.

### 4.3 Model II

In Model II, the cell is treated as an equilibrium cell and hence, the molecules are assumed to effuse from a flux source (FS) that is formed at the entrance of the orifice. As discussed in section 4.1, the Cosine law of effusion cannot be directly applied and the modified Cosine law of effusion derived in section 3.5.2.1 will be used for this model. The flux at every point on the platen has two components, the primary flux from the flux source and secondary flux from the walls of the orifice. The walls of the orifice receive
flux from the FS. The general setup of the cell and platen with flux components is shown in Figure 4.21.

In Figure 4.21, \( \hat{n}_f \) and \( \hat{n}_{pla} \) are the unit normals to the flux source and the platen respectively, and \( \theta_{tilt} \) is the angle of the tilt of cell from centre of platen. \( x_{pla} \) is the distance of the platen from origin which is located at the center of the opening of orifice. \( r_{pla} \) is the radius of the platen.

The process of generating points on the platen is exactly similar to the process described for Model I in section 4.2.1. The process of laying grid on FS is similar to process of laying grid on melt surface in Model I, except that the melt surface shape changes with \( \theta_{tilt} \) and level of the melt. In Model II, the FS is fixed for any angle of tilt and the angle between \( \hat{n}_f \) and cell axis remains \( \theta_f \). The process of laying grid on the wall of the orifice is similar to the process of laying grid on cell wall described for Model I in section 4.2.2, except that in Model I, the grid was laid on the entire surface, but in Model II, the grid is laid only on the orifice.

The process of calculating the flux on walls of orifice and total flux on platen is exactly similar to Model I except that the equations used in the process are different and are given below.

Flux on walls: 
\[
F_{-W-P}\_i = \sum_{j=1}^{n} \frac{(N+1)\Gamma \cos \varphi_j \cos \theta_{tilt} dA_{FS,j}}{2\pi r_j^2} \tag{4.25}
\]

Primary flux on platen: 
\[
F_{-Pri-P}\_i = \sum_{j=1}^{n} \frac{(N+1)\cos \varphi_j \cos \theta_{tilt} dA_{FS,j}}{2\pi r_j^2} \tag{4.26}
\]

Secondary flux on platen: 
\[
F_{-Sec-P}\_i = \sum_{j=1}^{n} \frac{(F_{-W-P}\_i) \cos \varphi_j \cos \theta_{tilt} dA_{wj}}{\pi r_j^2} \tag{4.27}
\]
where $N$ is the modifying parameter for the Cosine law of effusion and is determined by fitting with the experimental data. The remaining terms are similar to the terms described for Equations 4.21 to 4.23, except that the terms associated with the melt surface are now associated with the FS. From Equations 4.25 and 4.26, it is noted that the modified law is used only for molecules emitting from the FS and Equation 4.27 indicates that the molecules re-evaporating from the orifice walls, follows the Cosine law of emission. Another point to be noted is that if $N=1$ is substituted in Equations 4.25 and 4.26 the equations look exactly similar to the Equations 4.21 and 4.22 indicating that $N=1$ gives the Cosine law of evaporation. The process of obtaining the rotated flux is similar to the process described for Model I in section 4.2.5.
Figure 4.1 Geometry and dimensions of 10,000g SUMO cell

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Figure 4.2 General geometrical setup of the cell and platen for Model I
Figure 4.3 Picture depicting unphysical conditions of solutions of Equation 4.13 and 4.14
Figure 4.4 Pattern of points generated on the where flux will be computed

Figure 4.5 Pictorial description of Equations 4.3 and 4.4 for platen point generation
Figure 4.6 Cell surface viewed as a pack of circular grids.

Figure 4.7 Sampled points on the 2-d profile of cell
Figure 4.8 Pictorial view of axial grid line rotated to obtain the grid elements

Figure 4.9 A pictorial description of the angular relations between old and new points
Figure 4.10 The cell surface with grid elements

Figure 4.11 Pictorial description of the order of grid co-ordinates on the cell surface
Figure 4.12 Centroids and normals of each grid element on the cell surface

Figure 4.13 Pictorial representation of the geometry for obtaining the equation of the melt surface
Figure 4.14 Picture depicting un-physical conditions of solutions of Equation 4.13 and 4.14

Figure 4.15 Pictorial representation of the order of the co-ordinates for the grid points on the melt surface
Figure 4.16 Pictorial representation of the half cell used to calculate flux on the exposed cell wall
Figure 4.17 The four sections used for calculating wall flux

Figure 4.18 Pictorial description of the method for determining visible and invisible points of the melt surface for a point $P_1$ on the orifice wall.
Figure 4.19 Picture illustrating if the point is on the melt surface or not.

Figure 4.20 Limiting circles used in the flux calculation for a point on the platen
Figure 4.21 General setup of the cell and the platen used for Model II
CHAPTER 5

RESULTS AND DISCUSSION

5.1 Experimental

Experiments were conducted with the main body of the cell maintained at 1050°C and orifice was maintained at 20°C higher than the main body of the cell to avoid condensation at the orifice. The angle between the axis of the cell and normal to platen is 45° and the distance between the center of the platen and the center of opening of orifice is 32 inches (in). The platen was rotated azimuthally.

The thickness of gallium arsenide (GaAs) was measured at 7 locations on the wafer using X-Ray diffraction method described in section. It was assumed that the GaAs growth rate is controlled by the gallium (Ga) flux [68]. The thickness for each wafer is normalized to the maximum thickness on that wafer, which usually happens to occur at the center of the wafer. The results obtained for the normalized thickness on the three wafers are shown in Table I. The first column shows the radial location in inches on the wafer, the next three columns show the normalized thickness and the last column is the average of the normalized thickness for the three wafers.

The average normalized thickness is plotted in Figure 5.1 as a solid line and the minimum and maximum thickness at each radius is shown as error bars. The thickness at any location is determined by the amount of material deposited per unit area per unit time.
(flux or growth rate). Hence thickness is synonymous with the flux received at that location. In further discussions the term normalized thickness will be replaced by normalized flux.

The shape of the curve in Figure 5.1 indicates that the flux received at the center of the platen is more than the flux received at the edge of the platen. The flux variations for the three wafers are: 3.6207%, 3.8281% and 3.6701 respectively. The average flux variation for the three wafers is 3.7066%. The normalized flux variation is obtained theoretically using two numerical methods and the results for these models are discussed in the following sections.

5.2 Model I

In Model I, the crucible is treated as free evaporation type crucible and for complete details the reader is referred to section 4.2. The parameters which control the flux profile at the platen for this model are the angle between the cell and the platen, the melt level, and the distance between the cell and the platen. The observations made at each step of simulation will be described for a set of parameters and the experimental comparison is made at the end of the discussion.

A grid with 200 vertical and 80 horizontal sections was laid on the surface of the entire cell for a total of 16,000 grid elements. These numbers of sections were chosen to describe a smooth surface for the cell and at the same time to optimize the simulation time. A total of 3,205 grid elements were chosen on the surface of the melt. The flux calculated on the walls of the cell from the melt is shown in Figure 5.2. It is observed that the flux is concentrated at elements close to the top of the boundary of the melt as these
elements see the melt surface directly. The orifice receives very small amount of flux from the melt surface. In order to obtain the steady state wall flux distribution, multiple wall collisions were performed 34 times so that the change in flux on any grid element is less than 1%. The flux distribution after multiple wall collisions is shown in Figure 5.3. It is observed that the flux distributes itself onto all the grid elements and the conical portion of the main body of the cell has slightly more flux than the remaining parts of the cell wall. The reason for conical portion having more flux is due to more direct visibility of the portions of wall which had higher flux from the melt surface. It is also observed that the orifice also gets flux from the walls of the main body of the cell.

Having obtained the flux distribution inside wall of the cell, the flux profile was obtained on a platen whose radius is 8.72 in, (same as the experimental one). In order to account for the rotation of the platen, 40 concentric circles were laid on the platen and a total of 3,281 points on these concentric circles were considered for the flux calculation. For the details of the coordinate axis setup, the reader is referred to Figure 4.3. Before calculating rotated flux, un-rotated flux was calculated at all the points generated on the circles.

As discussed in Chapter 4, there are two components of flux, the primary and the secondary flux. The primary flux was calculated from the visible portions of the melt surface and the flux distribution is shown in Figure 5.4. It is observed that the un-rotated primary flux is symmetrical about the y-axis, and as we move along the y-axis from the center to the edge of the platen the flux reduces for the following two reasons, the first is, in Equation 4.21, the $\cos \varphi_j$ and $\cos \theta_{ij}$ reduces with increasing $\varphi_j$ and $\theta_{ij}$. The second reason is the amount of melt surface seen by the center point is greater than the edge
point along $y$-axis. It is also observed that the flux increases along the positive direction of $z$-axis for the following two reasons. The first reason is, in Equation 4.21, $\cos\theta_y$ and $\cos\theta_z$ increases as the position of point moves away from the center of the platen. The second reason is, $r_j$ reduces as the top end of platen is closer to cell opening.

The normalized un-rotated secondary flux was calculated from the visible parts of the cell wall and is shown in Figure 5.5. It can be observed that the flux is symmetric about $y$-axis and flux variation along the $y$-axis is less. The reason for this behavior is that as the receiving point moves toward the edge of platen, the portion of wall seen in the main body increases. The flux increases along the $z$-axis for the same reason as the primary flux.

The rotated primary flux is shown in Figure 5.6. It is observed that the flux is maximum at the center and decreases towards the edges of the platen. The rotated secondary flux is shown in Figure 5.7, and it can be observed that the flux is minimum at the center and increases towards the edges of the platen. The rotated total flux as shown in Figure 5.8 is constant on any circle. Therefore, in further discussions 3-D plots will be replaced by 2-D plots as shown in Figure 5.9. The experimental data is for normalized rotated total flux, in further discussions, the term total flux will be used instead of normalized rotated total flux.

In order to compare our results with experimental data, the total flux was computed for angle of tilt of $45^\circ$ and a platen distance of 32 in. As the experimental melt level is not available, melt levels of 5, 7, 9 and 11 in were used for simulation purposes. The flux profiles obtained for various melt levels are shown in Figure 5.10. The flux variation is calculated by the formula:
\[
\text{Flux Variation(\%)} = \frac{\text{Flux at the centre of the platen} - \text{Flux at the edge of the platen}}{\text{Flux at the centre of the platen}} \times 100
\] (5.1)

The flux variations calculated using Equation 5.1, for the various melt are given in Table II. As seen from Figure 5.10, as the melt level recedes into the cell, the variation in primary, secondary and total fluxes increases. The variation in primary flux increases because as the melt recedes the portion of the melt seen by the points on the edges of the platen reduces. The secondary flux variation is negative because the flux increases from center to the edge of platen. It is observed from Table II that the secondary flux helps in reducing the flux variation across the platen for any melt level. Since the total secondary flux is usually a fraction of the total primary flux, the total flux variation is dominated by the primary flux variation, as melt recedes.

The reduction in flux variation when melt recedes from 5 in to 7 in, is because, when the melt recedes along the conical section of the main body of the cell, its surface area of the melt increases, and edges of the platen see mostly constant surface area of melt. Once the melt recedes in to the cylindrical section, its surface area remains constant as it recedes and the edges of the platen will see less and less portions of the melt, resulting in an increase in the total flux variation.

Although simulations show that the melt level has a serious impact on the flux variation, in the experiment conducted on three wafers, even though after each run, the melt has receded, there was not much change in total flux variation. The strong dependence of flux variation on the melt level which is not observed in experiments makes Model I invalid, proving that free evaporation might not be the physics behind the effusion process. Thus this model is discounted a valid model.
5.3 Model II

In Model II, the emission is modeled as Knudsen type of effusion, in which a flux source (FS) is formed at the neck of the cell. For complete details of the emission process, the reader is referred to section 4.2. The parameters which control the flux profile at the platen are angle of tilt of the cell and the distance between the platen. The melt level is no longer important as it is assumed that flux emitted by the virtual FS does not depend on the melt level. The parameters which control the behavior of the model are discussed below with simulation results at each stage.

A grid with 100 vertical and 40 horizontal sections was laid on the orifice section of the cell for a total of 4,000 grid elements. A square grid of 0.05 in size was laid on the FS giving a total of 761 grid elements. The first concern for modeling is the position of the FS in the orifice. The total flux on the platen was evaluated for different positions of FS in the orifice and the results are tabulated in Table III. The simulations were performed without modifying the Cosine law of effusion (which is the same as substituting N=1 in equations 4.25 and 4.26) and experimental parameters for angle of tilt, the distance of platen from cell and radius of the platen.

As the orifice is symmetrical about the x-axis, a 2-d profile of the orifice as shown in Figure 5.11 will be used for the discussions. The origin is located at the opening of the orifice also referred to as the mouth of the orifice. The FS is assumed to form in the neck of the orifice, which extends from 3.1 in to 3.5 in, as shown in Figure 5.11. When the location of the FS is 3.1 in, with respect to the origin, the edges of the platen will see the whole of FS as the only limiting circle is at the mouth, but as the location moves deeper
into the neck of the orifice, the neck region between 3.1in and the present location obstructs the view of some points on the edge of platen. As the FS moves deeper into the neck, lesser portions of the FS are seen by the edge of platens than the center and hence, the total flux variation increases. When the location goes much deeper, the FS will be in the conical section of the main body of the cell. The center of the platen will not be able to see the edges of the VFS located in conical section. But the edges of the platen will be able to see certain portion of the edges of the FS and hence, the flux variation decreases as is evident from the data in Table III for location 3.7 in.

It is observed from data in Table III that, neither of the locations for FS will be able to match experimental flux variation of 3.7066% and hence the modified Cosine law of effusion has to be used. In order to be able to make the model general for any cell the uncertainty in choosing correct location for FS has to be resolved and hence, the thumb rule is to choose the VFS at that location in neck which results in minimum radius for the FS. For the present cell, the location was chosen as 3.3 in at which the radius is 0.75 in.

Having fixed the location for FS, the simulations were performed for different values of N and the results are tabulated in Table IV. Multiple wall collisions on the orifice were simulated at each stage. For the present orifice shape, the collisions were continued till the change in areal rate of emission (flux) for any wall grid element is less than 0.1%. The number of iterations required for any value of the exponent for the modified Cosine law \((\cos^N \varphi)\) remained constant at 27. The distribution of flux on the walls before and after multiple wall collisions is shown in Figure 5.12. It can be observed that flux from melt peaks on wall elements close to the FS before multiple wall collisions. But after
multiple wall collisions, the flux distribution on the walls smoothens out and falls gradually towards the opening of the orifice.

From Table IV, it is observed that the total flux variation increases as N increases. It is also observed that the primary flux variation and the reason is that the molecules are increasingly focused toward the centre of the platen. The secondary flux variation remains constant and the reason is that due to multiple wall collisions, the distribution of flux on walls does not change with N. The flux variation for N=1.9, matches well with the experimental data and hence will be used in further discussion.

The un-rotated primary and secondary flux are shown in Figures 5.13 and 5.14. The rotated flux components are shown in Figure 5.15. The flux is not normalized to provide a clear picture regarding the ratio of primary to secondary flux. It can be observed that primary flux is nearly 4 times more than the secondary flux. The shape of the secondary flux profile shows a maximum at the center and minimum at the edge because the center sees the entire orifice wall but the edge of platen sees only a part of the orifice wall.

The simulated and experimental normalized total fluxes are shown in Figure 5.16. It can be observed that there is good agreement between both the results. The agreement in results for Model II proves that the evaporation is Knudsen effusion but with a higher value for the exponent N. This shows that 10,000g SUMO cell exhibits more focusing effect than that predicted by Cosine law of effusion.
5.4 Design considerations for the cell

The new model developed can be used to study the effect of parameters such as angle of the tilt, the distance of the platen and shape of the orifice, which can help in improving flux uniformity. One other important parameter which can be investigated with the help of this model is efficiency.

5.4.1 Efficiency

Efficiency represents the amount of material that is actually used for growing the epilayer and is given by:

\[ Efficiency(\%) = \frac{\text{Total flux within the user defined platen}}{\text{Total flux within the virtual platen}} \times 100 \]  \hspace{1cm} (5.2)

Only a part of the flux effusing from the cell is received by the platen and the rest will be received by the deposition chamber walls. To capture the flux effusing from the cell a larger platen is employed for the simulation purpose. The larger platen does not represent the actual size of the platen and hence is termed as virtual platen.

To calculate total flux received by the platen and the virtual platen the following procedure is adopted. As discussed in section 4.2.1, the platen was represented by a set of concentric circles. The flux was evaluated at the points on each circle and averaged to give rotated flux on that circle. The process was repeated for each circle to get the flux profile on the entire platen. The concentric circles on the platen represent annular rings and the flux in each annular ring is constant. The flux in the annular ring is given by the product of the area of the ring and the flux received by the inner circle of the ring. The area of the ring is given by the product of circumference of the inner circle and the width of the ring, which is nothing but the spacing between the circles forming the ring. Based on the above discussion the equation for flux in any \(i^{th}\) annular ring is given by:
where \( r_i \) is the radius of the inner circle of the annular ring and is given by Equation 4.1. The spacing between the circles forming annular ring is given by dividing radius of actual platen, \( r_{pla} \), by the number of circles considered on the whole platen, \( nr \). \( F_{ci} \) is the rotated flux on the inner circle of the ring.

The total flux collected by the platen is given by adding up the flux of all the annular rings. Combining Equations 4.1 and 5.3 the equation for the total flux collected on the platen is given by:

\[
F_{pla} = \sum_{i=1}^{n} 2\pi i \left( \frac{r_{pla}}{nr} \right)^2 F_{ci}
\]

where \( n \) is the number of annular rings. The total flux collected on the virtual platen is given by replacing \( r_{pla} \), with the radius of the virtual platen (\( r_{vpla} \)).

The radius of the virtual platen is chosen in such a way that the flux on the edges of the virtual platen is nearly zero. In other words the platen will capture almost all of the flux effused by the cell. For the present system setup, a platen of radius 50 in assured that the flux at the edge of the platen reduces to 1.7% of the flux at center of the platen as shown in Figure 5.17. The efficiency thus calculated for the experimental setup is 17.9%.

5.4.2 Tilt of the cell

The angle of tilt of the cell, \( \theta_{tilt} \) was changed from 0° to 80° in steps of 5° and the flux variation and efficiency were obtained. The plots obtained are shown in Figure 5.18. It is observed that as angle increases the flux variation decreases and then increases. The critical angle, at which the flux variation is minimum, is 52° and the corresponding flux
variation is 0.45236 %. The efficiency decreases as the angle increases and at the critical angle the efficiency is 16%. The important observation is that by changing the original angle of tilt from 45° to 52°, the flux variation dramatically decreases but the efficiency does not decrease much.

5.4.3 Distance between the cell and platen

The distance between the cell and the platen was changed from 0 in to 50 in, in steps of 5 in and the plot of efficiency and flux variation is shown in Figure 5.19. It is observed that at 0 in, the flux variation and efficiency are 100%, the reason for the observed behavior is that, the platen is at the mouth of the cell and hence the whole material is collected within a radius of 5 in. It can be observed that till 10 in, the flux variation drops slower than the efficiency, but from 10 in to 20 in the flux variation drops faster than the efficiency and after 25 in the change is slower for both efficiency and flux variation. The choice of distance depends on the user’s priority of efficiency and or uniformity. It is suggested that the distance of 20 in is a good compromise for obtaining a reasonable flux variation of 10.8% and efficiency of 36%.

Usually in an MBE system used in industry, the distance of platen and angle of tilt of cell are fixed and hence, the geometry of the cell plays an important role in controlling the efficiency and flux variation. A direct way of reducing flux variation is to make the diameter of the neck of the orifice smaller, as the orifice is now closer to the ideal Knudsen orifice, the N parameter approaches to 1. But reducing the neck diameter also reduces the rate at which the material is grown and hence, modification of N should be done only in cases where uniformity is extremely important than the growth rate. Another way of controlling the required parameters is by changing the shape of the orifice. For the
present cell, two parameters are used to model the geometry of the orifice as shown in Figure 5.20. $\theta_{ori}$ is the angle of opening of the orifice and $x_{ori}$ is the length of the orifice. For the present cell, $\theta_{ori}$ is $18.435^\circ$ and $x_{ori}$ is 3.3 in.

Simulations were performed for different combinations of length of the orifice and the angle of the opening and the results are tabulated in Table V. The lengths and angles were chosen to preserve the general profile of the orifice and change only the size. It can be observed that if the length of the orifice is increased, the efficiency increases. The reason for this behavior is that the increase in surface area of the walls which contribute more secondary flux. When the length of the orifice increases the angle of orifice reduces if the radius of the mouth of the cell is kept and hence, flux variation increases. Hence when the length is increased care should be taken to change the radius of the mouth such that the angle remains constant.

It is observed that if the angle of the orifice is increased, the flux variation reduces. The reason for this behavior is the unobstructed view of FS to all the points on the platen. As the angle of orifice increases, the efficiency decreases as the flux on the walls of the orifice from the melt surface reduces and also more flux from VF effuses towards the unwanted portions of platen. It should be noted that the increase of the angle after a certain critical value will not reduce the flux variation because at the critical angle, all points on the platen have complete view of the FS and increasing the angle does not change the view.
Table I Table showing experimental thickness data obtained for three different wafers. The cell used was 10,000g SUMO cell and it was placed at a distance of 32 in from the platen and at angle of 45° to the platen.

<table>
<thead>
<tr>
<th>Radius (in)</th>
<th>Wafer 1</th>
<th>Wafer 2</th>
<th>Wafer 3</th>
<th>Average</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.01388</td>
<td>1.01507</td>
<td>1.01138</td>
<td>1.01344</td>
</tr>
<tr>
<td>1.79</td>
<td>1.01309</td>
<td>1.01110</td>
<td>1.01257</td>
<td>1.01226</td>
</tr>
<tr>
<td>3.6</td>
<td>1.00837</td>
<td>1.00555</td>
<td>1.00299</td>
<td>1.00563</td>
</tr>
<tr>
<td>5.37</td>
<td>1.00046</td>
<td>1.00674</td>
<td>1.00419</td>
<td>1.00380</td>
</tr>
<tr>
<td>7.17</td>
<td>0.98704</td>
<td>0.98533</td>
<td>0.99461</td>
<td>0.98899</td>
</tr>
<tr>
<td>8.72</td>
<td>0.97717</td>
<td>0.97621</td>
<td>0.97426</td>
<td>0.97588</td>
</tr>
</tbody>
</table>

Table II Flux variations obtained from Model I for different melt levels. The orientation, shape of the cell and the size of the platen are same as the experimental setup.

<table>
<thead>
<tr>
<th>Melt Level (in)</th>
<th>5</th>
<th>7</th>
<th>9</th>
<th>11</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Flux Variation (%)</td>
<td>1.2627</td>
<td>1.01</td>
<td>4.943</td>
<td>23.732</td>
</tr>
<tr>
<td>Primary Flux Variation (%)</td>
<td>3.8746</td>
<td>3.4116</td>
<td>8.7076</td>
<td>33.226</td>
</tr>
<tr>
<td>Secondary Flux Variation (%)</td>
<td>-0.1586</td>
<td>-0.5129</td>
<td>-2.9921</td>
<td>-15.348</td>
</tr>
</tbody>
</table>

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Table III Flux variations obtained using Model II for different positions of flux source in the orifice. The orientation, shape of the cell and the size of the platen are same as the experimental setup.

<table>
<thead>
<tr>
<th>Location of VFS (in)</th>
<th>3.1</th>
<th>3.2</th>
<th>3.3</th>
<th>3.4</th>
<th>3.5</th>
<th>3.6</th>
<th>3.7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Radius of VFS (in)</td>
<td>0.7702</td>
<td>0.755</td>
<td>0.75</td>
<td>0.755</td>
<td>0.79</td>
<td>0.796</td>
<td>0.834</td>
</tr>
<tr>
<td>Total Flux Variation (%)</td>
<td>0.64608</td>
<td>0.83939</td>
<td>1.8365</td>
<td>2.3529</td>
<td>3.037</td>
<td>3.2911</td>
<td>2.6194</td>
</tr>
</tbody>
</table>

Table IV Flux variations, for different values of N parameter used to modify cosine law in Model II. The orientation, shape of the cell and the size of the platen are same as the experimental setup.

<table>
<thead>
<tr>
<th>N</th>
<th>Primary Flux Variation (%)</th>
<th>Secondary Flux Variation (%)</th>
<th>Total Flux Variation (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
<td>2.3032</td>
<td>0.70911</td>
<td>1.8365</td>
</tr>
<tr>
<td>1.2</td>
<td>2.7808</td>
<td>0.70903</td>
<td>2.2314</td>
</tr>
<tr>
<td>1.3</td>
<td>3.0187</td>
<td>0.70904</td>
<td>2.4349</td>
</tr>
<tr>
<td>1.4</td>
<td>3.256</td>
<td>0.70905</td>
<td>2.6417</td>
</tr>
<tr>
<td>1.5</td>
<td>3.4926</td>
<td>0.70906</td>
<td>2.8515</td>
</tr>
<tr>
<td>1.6</td>
<td>3.7287</td>
<td>0.70907</td>
<td>3.0638</td>
</tr>
<tr>
<td>1.7</td>
<td>3.9641</td>
<td>0.70908</td>
<td>3.2785</td>
</tr>
<tr>
<td>1.8</td>
<td>4.1989</td>
<td>0.70909</td>
<td>3.4951</td>
</tr>
<tr>
<td>1.9</td>
<td>4.4331</td>
<td>0.70909</td>
<td>3.7143</td>
</tr>
</tbody>
</table>
Table V Flux variation obtained using Model II for various shapes of the orifice. The orientation of the cell and size of platen are same as the experimental setup

<table>
<thead>
<tr>
<th>$x_{ori}$</th>
<th>$\theta_{ori}$</th>
<th>Total Flux Variation (%)</th>
<th>Efficiency (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.05</td>
<td>19.832</td>
<td>3.7137</td>
<td>14.981</td>
</tr>
<tr>
<td>3.1148</td>
<td>26.4344</td>
<td>2.4428</td>
<td>14.08</td>
</tr>
<tr>
<td>3.2152</td>
<td>22.4349</td>
<td>2.9282</td>
<td>15.432</td>
</tr>
<tr>
<td>3.2596</td>
<td>20.4349</td>
<td>3.2384</td>
<td>16.289</td>
</tr>
<tr>
<td>4.05</td>
<td>16.7486</td>
<td>3.7591</td>
<td>19.686</td>
</tr>
<tr>
<td>4.8</td>
<td>15.5714</td>
<td>3.7864</td>
<td>22.072</td>
</tr>
<tr>
<td>6.2412</td>
<td>16.0380</td>
<td>3.2416</td>
<td>23.769</td>
</tr>
<tr>
<td>6.3</td>
<td>14.038</td>
<td>3.8458</td>
<td>26.642</td>
</tr>
<tr>
<td>6.9877</td>
<td>21.3591</td>
<td>2.4133</td>
<td>19.288</td>
</tr>
<tr>
<td>7.1613</td>
<td>17.3591</td>
<td>2.9058</td>
<td>23.226</td>
</tr>
</tbody>
</table>
Figure 5.1 Average Experimental thickness profile obtained using X-ray diffraction techniques. The cell used was 10,000g SUMO cell placed at a distance of 32 in and angle of 45° to the wafer.
Figure 5.2 Distribution of flux from the melt surface on the wall of the cell.

Figure 5.3 Distribution of flux on the walls of the cell after multiple wall collisions
Figure 5.4 Un-rotated normalized primary flux profile obtained using Model I. The melt level used is 9 in. The orientation, shape of the cell and the size of the platen are same as the experimental setup.

Figure 5.5 Un-rotated normalized secondary flux profile obtained using Model I. The melt level used is 9 in. The orientation, shape of the cell and the size of the platen are same as the experimental setup.
Figure 5.6 Rotated normalized secondary flux profile obtained using Model I. The melt level used is 9 in. The orientation, shape of the cell and the size of the platen are same as the experimental setup.

Figure 5.7 Rotated normalized secondary flux profile obtained using Model I. The melt level used is 9 in. The orientation, shape of the cell and the size of the platen are same as the experimental setup.
Figure 5.8 Rotated normalized total flux profile obtained using Model I. The melt level used is 9 in. The orientation, shape of the cell and the size of the platen are same as the experimental setup.

Figure 5.9 2-D flux profiles of normalized total, primary and secondary flux components obtained using Model I. The melt level used is 9 in. The orientation, shape of the cell and the size of the platen are same as the experimental setup.

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Figure 5.10 2-D flux profiles of normalized total, primary and secondary flux components obtained using Models I for various melt levels. The experimental data is also shown.

Figure 5.11 2-D profile of orifice section of the cell

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Figure 5.12 Flux on the walls of the orifice with and without multiple wall collisions in Model II.

Figure 5.13 Un-rotated normalized primary flux profile obtained using Model II. The orientation, shape of the cell and the size of the platen are same as the experimental setup.
Figure 5.14 Un-rotated normalized secondary flux profile obtained using Model II. The orientation, shape of the cell and the size of the platen are same as the experimental setup.

Figure 5.15 2-D flux profiles of normalized total, primary and secondary flux components obtained using Model II. The orientation, shape of the cell and the size of the platen used are same as experimental setup.
Figure 5.16 Comparison of experimental flux profile and total flux obtained by Model II.

Figure 5.17 Flux profile on a virtual platen of 50 in used for efficiency calculations. The orientation and shape of cell are same as experiment. The profile is obtained by Model II.
Figure 5.18 Flux variation and efficiency change with angle of tilt of cell $\theta_{\text{tilt}}$ obtained using Model II.

Figure 5.19 Flux variation and efficiency change as with platen distance obtained using Model II.
Figure 5.20 Pictorial description of parameters used to define the shape of the orifice.
CHAPTER 6

CONCLUSION AND RECOMMENDATIONS

6.1 Conclusion

In this study, the advantages of MBE as a deposition technique were presented. The uses of MBE in semiconductor research and industry were discussed. The problems associated with industrial MBE systems were identified. The problem of non-uniformity in thickness of material grown was identified as a major problem. The parameters which effects the thickness uniformity were identified as, the orientation of the source (cell) with respect to the platen and the shape of the cell. A computer based simulation tool was developed to study the effect of these parameters.

To develop the simulation tool, the physics behind the emission process was understood. Depending on the shape of the cell, two types of emission process were identified. If the diameter of the opening of the cell is equal to or greater than the diameter of the source material, then the process of emission was identified as Langmuir or free evaporation. If the diameter of the opening of the cell is less than the diameter of the source material, then the emission was identified as Knudsen effusion.

Based on the type of emission, two models were developed for the simulation tool. Model I is for free evaporation and Model II is for Knudsen effusion. The
programming for both the models was based on numerical computation techniques. The results obtained by simulation were compared to experimental data available for 10,000g SUMO cell. The type of emission for 10,000g SUMO cell was identified as Knudsen effusion. The cosine law of effusion developed by Knudsen for research cells, when employed for Model II, did not match the experimental results. The reason for this observation was identified as the radius of the opening of the 10,000g cell, which was larger than the radius of research cells. Hence, a modified Cosine law of effusion was developed for Model II. The results obtained for Model II with the modified cosine law of effusion are in good agreement with the experimental data.

The new model developed was used to study the effects of various parameters which affect the uniformity in thickness. The simulation tool could also provide extra information like the efficiency of material usage. The observations are presented in the following paragraphs.

The orientation of the cell with respect to the platen is controlled by two parameters. They are: the angle of tilt of the cell (θ_{tilt}) with respect to the platen and the distance of the cell from the platen (x_{platen}). It was observed that as θ_{tilt} was increased from 0° (perpendicular) to 90° (parallel), there exists a critical angle at which the flux variation (non-uniformity in thickness) is minimum. The efficiency of material usage decreased with increase in θ_{tilt}. It was observed that as x_{platen} is increased, the flux variation and the efficiency decrease.

The 10,000g Sumo cell has a conical orifice attached to the opening of the cell. It was observed that the shape of this orifice has serious effect on the flux variation and efficiency. It was observed that as angle of cone increases, the flux variation reduces.
initially and then remains constant. It was also observed that the efficiency decreases with increasing angle of cone. It was observed that as length of cone increases, the efficiency increases and the flux variation remains constant.

This simulation tool provides a simple and cost effective way of designing new cells to meet the requirements of the industry standard MBE system.

6.2 Recommendations

The results of the model suggest that there is scope for improving the design of GEN 2000 MBE system which employs 10,000g SUMO cells. It is recommended to change $\theta_{oh}$ from $45^0$ to $52^0$ as this reduces the flux variation from $3.7\%$ to $0.45\%$ without much loss in efficiency. It is recommended to change the orifice shape according to the requirement of the user. Some of the designs presented in Table IV will aid the user in choosing the shape of the orifice.

To validate the modified cosine law, it is recommended to obtain experimental results for varying diameter of the cell and check if the results match with simulation. If the law is valid it is recommended that from the same experimental data an expression for value of modifying parameter $N$ be obtained. In the present model the shape of the cell is defined manually. It is recommended to automate the process by linking the available tool to commercially available software's like AUTOCAD etc.

The present model is developed for pyrolytic boron nitride (PBN) cells which effuse gallium species. In order to model cells made of different materials and effusing different species, it is recommended to include surface diffusion into the present model. The present model is valid for 10,000g cell operated at a temperature
of $1070^\circ$. In order to model cells operating at different temperatures it is recommended to include specular reflection into the present model.
I) Evaporative processes
   1) Molecular-beam epitaxy (MBE)
   2) Electron-beam evaporation
   3) Reactive evaporation
II) Glow discharge processes
   1) Sputtering
      a) Diode sputtering
      b) Reactive sputtering
      c) Bias sputtering (ion plating)
      d) Magnetron sputtering
      e) Ion beam deposition
      f) Ion beam sputter deposition
      g) Reactive ion plating
      h) Cluster beam deposition (CBD)
   2) Plasma Processes
      a) Plasma-enhanced CVD
      b) Plasma oxidation
      c) Plasma anodization
      d) Plasma polymerization
      e) Plasma nitridation
      h) Plasma reduction
      f) Microwave ECR plasma CVD
      h) Cathodic arc deposition
III) Gas phase chemical processes
   1) Chemical Vapor Deposition (CVD)
      a) CVD epitaxy
      b) Atmospheric-pressure CVD (APCVD)
      c) Low-pressure CVD (LPCVD)
      d) Metalorganic CVD (MOCVD)
      e) Photo-enhanced CVD (PHCVD)
      f) Laser-induced CVD (PCVD)
      g) Electron-enhanced CVD
      h) Ion implantation
2) Thermal Forming Processes
   a) Thermal oxidation
   b) Thermal nitridation
   c) Thermal polymerization

IV) Liquid phase chemical processes
1) Electro Processes
   a) Electroplating
   b) Electroless plating
   c) Electrolytic anodization
   d) Chemical reduction plating
   e) Chemical displacement plating
   f) Electrophoretic deposition
   g) Liquid phase epitaxy
2) Mechanical Techniques
   a) Spray pyrolysis
   b) Spray-on techniques
   c) Spin-on techniques
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Publications:

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Flux Profile modeling using Numerical Methods

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Committee member, Dr. Sahjendra Singh, Ph. D.
Graduate College Representative, Dr. Laxmi P. Gewali, Ph. D.