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Line segment simulation of sputtered thin film growth over VLSI topography

by

Abdisalam Sheikh-Omar Mo'allim

A thesis submitted to the

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Master of Engineering

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Department of Electronics

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Studied and Research acceptance of this thesis
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growth over a topography for VLSI design
submitted by Abdisalam Sheikh-Omar Mo'allim
in partial fulfilment of the requirement for
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Abstract

SIMPROF is a line segment simulator written to simulate thin film deposition on VLSI topography. The fundamental data structure is a linked list of nodes representing the surface as a string of segments. Each node contains information on the node position, normal and growth angle. The flux striking the surface is assumed to create a concentration of Physiosorbed adatoms whose deposition on the surface can be described by a diffusion equation. The effect of the flux shadowing is determined to obtain a correct deposition profile.

A very limited version of SIMPROF existed prior to this work and accounted only for a simple 2D simulations. The original SIMPROF was rewritten and extended and a new 3D version was developed. The new version of SIMPROF accounts for diffusive, specular and resputtering/re-emission models. New and effective surface advancing techniques were incorporated into SIMPROF to correctly simulate the complex growth of convex and concave corners. The consideration of the density variations in the deposited film is also considered within the program. As the surface grows new nodes are added or removed to maintain the integrity of the topography surface. When the required film is grown a question that arises is how this simulated film compares to a real films. To verify SIMPROF as a valid simulator we compare its simulation results to experimental films and to other validated simulators such as SIMBAD. A comparison with SIMBAD provided a strong motivation for the development of SIMPROF. Situations sometimes appear when algorithmic problems are difficult to separate from physical effects and two distinct simulation approaches can be used as a tool for investigation.

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Chapter 1 1

1.1:	Introduction.....	1
1.2:	Role of metallization in VLSI.....	3
1.3:	Multilevel Metallization.....	5
1.4:	Deposition methods.....	6
1.4.1	Thermal evaporation.....	8
1.4.2	Chemical vapour deposition.....	9
1.4.3	Sputtering processes.....	10
1.4.3.1	Bias sputtering.....	12
1.4.3.2	Directed sputtering.....	13
1.5:	Thin film properties.....	15
1.6:	Growth mechanics.....	16
1.7:	Nucleation and growth.....	17
1.8:	Film structure.....	18
1.9:	Electrical properties of thin films.....	19
1.10:	Contacts and vias.....	20
1.11:	Barrier and encapsulation layers.....	21
1.12:	Step coverage and bottom coverage.....	24
1.13:	Topography of vias and contacts.....	26
1.14:	Simulators.....	28
1.15:	Types of models.....	30
1.15.1	Molecular Dynamics.....	31
1.15.2	Atomistic Monte Carlo Model.....	32
1.15.3	String algorithm.....	32
1.15.4	Ballistic deposition.....	33
1.16:	Motivation for SIMPROF.....	34

Chapter 2 37

2.1:	An outline of SIMPROF.....	37
2.2:	Initial surface representation.....	41
2.3:	Surface data structures	44
2.4:	Incident flux source representation in SIMPROF (2D and 3D)	45
2.5:	Incident flux Distribution	50
2.6:	Visibility issues.....	52
2.6.1	Two dimensional visibility	52
2.6.2	Quasi_three dimensional visibility	54
2.7:	Visibility testing procedures in SIMPROF.....	60
2.7.1	Two dimensional visibility testing criteria	60
2.7.2	Three dimensional visibility testing criteria	65
2.8:	Flux calculations with unity sticking coefficient (2D and 3D).....	76
2.9:	Flux reflection models	80
2.10:	Flux calculations with reflection in 2D using iteration.....	84
2.11:	Flux data structure	86
2.12:	Surface diffusion.....	87
2.13:	Surface evolution	91

Chapter 3 92

3.1:	Surface movement algorithms	92
3.2:	Film growth modeling	95
3.3:	Low mobility	95
3.4:	High mobility.....	98
3.5:	Deposition over topography.....	99
3.6:	Uniform deposition	100
3.7:	SIMPROF's growth modeling.....	101

3.7.1	Surface evolution toward node normal	104
3.7.2	Film growth with respect to average flux direction	108
3.7.3	Thin film growth with respect to segment mass weighted average direction	110
3.8:	Failure of the attempted growth modeling.	114
3.9:	Basic algorithms for advancing surface.	115
3.9.1	Flat surface	115
3.9.2	Convex surface	116
3.9.3	Concave surface	118
3.10:	Film density	123
3.11:	Reliability of the model	124

Chapter 4 126

4.1:	Validation strategy.	126
4.2:	SIMBAD.	127
4.3:	Level set	128
4.4:	Verification procedure.	128
4.5:	SIMPROF's validation	132
4.5.1	Validation of SIMPROF in 2D through variation of deposition width and constant sticking coefficients.	138
4.5.2	Validation of SIMPROF in 2D through variation of sticking coefficients and constant deposition width.	141
4.5.3	Validation of SIMPROF In 3D under unity sticking coefficient and varying deposition width	145
4.6:	Verification of SIMPROF with respect to experimental films.	146
4.7:	Verification of SIMPROF using high aspect ratio topographies	152
4.8:	Verification of SIMPROF by using experimental films on overhang structure	154

Chapter 5	 159
------------------	------------------

5.1: Conclusion	159
-----------------------	-----

5.2: Recommendation for further work	161
--	-----

BIBLIOGRAPHY:	163
----------------------------	------------

Fig 1.1	a) Exponential growth of the number of components per IC chip (b) Exponential decrease of the minimum device dimension	2
Fig 1.2	A cross-sectional view of a single MOS device illustrating two level metallization process.	6
Fig 1.3	Schematic depiction of a) Standard sputtering system b) Long throw sputtering system and c) Collimated sputtering system.	14
Fig 1.4	Via and contact schemes	23
Fig 1.5	Encapsulation schemes.	24
Fig 1.6	a) Depiction of step coverage of via and b) Depiction of aspect ratio of via.	25
Fig 1.7	a) Metal discontinuity caused by steep via hole because of shadowing effect and b) Improved step coverage using a tapered profile.	27
Fig 1.8	Contact scheme of stacked via.	28
Fig 1.9	Contact scheme of staggered vias	29
Fig 1.10	a) Simulation output from SIMPROF and b) Simulation output from SIMBAD over a trench with a thickness of 1mm and distribution width of 10.	36
Fig 2.1	Flow chart for 2D simulation model.	39
Fig 2.2	Flow chart for 3D simulation model.	40
Fig 2.3	a) Surface created from Table 1.1 definition of topography b) Surface created from Table 1.2 definition of topography and c) Surface created from Table 1.3 definition of topography.	43
Fig 2.4	Depiction of data structure arrangement.	45
Fig 2.5	Flux contribution from source line to specific substrate node.	47
Fig 2.6	Flux contribution from plane source to specific substrate segment: we only considered one loop of the plane source for simplicity.	49
Fig 2.7	Angular distribution of the sputtered atoms generated by SIMSPUD for Ti.	51
Fig 2.8	A cosine angular flux distribution from source point.	51

Fig 2.9	a) Vertical flux to vertical segment b) Vertical flux to any segment except vertical segment c) Any flux except vertical one to vertical segment and d) All slanted fluxes to slanted segments.	54
Fig 2.10	General half cut surface view that receives incident film having either disc, cylindrical or conical shapes.	56
Fig 2.11	Graphical representation of shadowing and non-shadowing effects of discs (flat surfaces).	57
Fig 2.12	Graphical representation of shadowing and non-shadowing effects of cylindrical segments.	58
Fig 2.13	Graphical representation of shadowing and non-shadowing effects of conical segments.	59
Fig 2.14	Depiction of 2D shadowing effect, dotted flux lines are shadowed.	60
Fig 2.15	Visibility testing criteria of vertical segment and flux line a) Shadowing is not possible and b) Shadowing is possible.	62
Fig 2.16	Visibility testing criteria of slanted segment and slanted flux line for 2D a) Shadowing is not possible and b) Shadowing is possible.	64
Fig 2.17	Illustration of non shadowing effect for 3D when both source and target are above or below of the shadowing surfaces.	65
Fig 2.18	Flux shadowing properties of a Disc where a) Flux is not shadowed and b) Flux is shadowed.	66
Fig 2.19	Non shadowing properties of cylindrical surfaces.	67
Fig 2.20	Shadowing properties of cylindrical surfaces.	68
Fig 2.21	Illustration of conical non shadowing surface properties.	69
Fig 2.22	Illustration of conical shadowing surface properties.	70
Fig 2.23	Implicit visibility property of cylindrical surfaces.	74
Fig 2.24	Implicit visibility property of conical surfaces.	75
Fig 2.25	a) Determination of y_{min} and b) Determination of r_{sur} . The line marked with 1 and similar lines use r_{sur1} others use r_{sur2}	76
Fig 2.26	Depiction of how the flux transport from source segment to substrate	

	segment is calculated.	80
Fig 2.27	Thin film deposition models a) All incident flux sticks to the surface (Unity sticking), b) Diffusive-lossy model, c) Diffusive-chemical model, d) specular_lossy model, e) Specular model and f) Resputtering model. ...	84
Fig 2.28	Central difference approximation.	90
Fig 3.1	Illustration of the entropy condition of Huygens' principle.	93
Fig 3.2	Columnar structure of a film grown from obliquely incident flux	97
Fig 3.3	Simulated film from SIMBAD.	97
Fig 3.4	Nodes move in the direction of the incident flux	98
Fig 3.5	A smoother columnar film structure grown from obliquely incident flux at high diffusion.	99
Fig 3.6	Dependence of deposition on topography structure and direction of flux. a) Vertical wall trench b) Depiction of corner growth of a. and c) Sloped wall trench.	100
Fig 3.7	Uniform deposition through surface topography.	101
Fig 3.8	Simulated films from SIMPROF a) With overlaps and b) With overlaps being cleaned up.	103
Fig 3.9	Depiction of how node normal is calculated.	105
Fig 3.10	a) How segment normal is determined by using isolated segment and b) Depiction of growth direction with respect to growth angle.	105
Fig 3.11	Simulation output using node normal growth direction at distribution angle of 1° and unity sticking a) Uniform growth b) High diffusion growth c) Zero diffusion growth d) The expected output for zero diffusion growth and e) Depiction of why part c of the Fig 3.11 failed	107
Fig 3.12	Relation between flux distribution over bins and average flux direction.	109
Fig 3.13	Simulation outputs from SIMPROF using average flux direction at distribution width of 1° and a) Zero diffusion simulation output b) Highly diffusive.	110
Fig 3.14	This figure depicts how weighted mass average is calculated a) When mt_2 is	

	zero b) When mt_1 and mt_2 are not zero for concave surface and c) When $mt_1 = mt_2$ for convex surface.	112
Fig 3.15	Depiction of deviated and corrected growth angles.	113
Fig 3.16	Simulation output using weighted mass growth direction at distribution angle of 1° and unity sticking a) Uniform growth b) High diffusion growth c) Zero diffusion growth and d) The expected output of c.	114
Fig 3.17	Model of modified weighted mass average growth angle for flat surface.	116
Fig 3.18	Expected growth from modified weighted mass average growth angle for convex surface a) When $mt_1 = mt_2$ b) When $mt_2 < mt_1$ and c) When $mt_2 \ll mt_1$	118
Fig 3.19	Expected growth from concavely formed corner of a growing film.	121
Fig 3.20	Flux geometry depicting how the surface is advanced in concave corners. ...	121
Fig 3.21	Simulation outputs from SIMPROF with a1) $Sc=1$, Dep Width $=1^\circ$ at zero diffusion a2) $Sc=0.5$, Dep Width $=1^\circ$ at zero diffusion a3) $Sc=1$, Dep Width $=1^\circ$ with diffusion b1) $Sc=1$, Dep Width $=90^\circ$ at zero diffusion b2) $Sc=0.5$, Dep Width $=90^\circ$ at zero diffusion b3) $Sc=1$, Dep Width $=90^\circ$ with diffusion c1) $Sc=1$, Dep Width $=180^\circ$ at zero diffusion c2) $Sc=0.5$, Dep Width $=180^\circ$ at zero diffusion c3) $Sc=1$, Dep Width $=180^\circ$ with diffusion and e) uniform deposition.	122
Fig 3.22	Simulated films from SIMPROF using distribution width of 60° with $Sc = 0.5$ a) thin film depiction on stepped topography b) Exhibition of density variation of (a), c) Thin film depiction on slanted topography and d) Demonstration of density variation of (c).	124
Fig 4.1	Vertically deposited films a) Simulation from SIMPROF with no diffusion, b) and c) Simulations from SIMPROF and SIMBAD at low diffusion, and c) Simulation using level set program.	130
Fig 4.2	Uniformly deposited films a) Simulation using SIMPROF b) Simulation using SIMBAD and c) Simulation using the level set program.	131

Fig 4.3	Illustration of how SIMPROF and SIMBAD simulation outputs in 2D are comparable to each other a) and b) Are SIMPROF and SIMBAD simulations respectively at a distribution width of 1° and unity sticking coefficient and c) and d) Are simulation outputs from both simulators respectively at a distribution width of 45° and unity sticking coefficient. 134
Fig 4.4	Illustration of how SIMPROF and SIMBAD simulation outputs in 2D are comparable to each other a) and b) Are SIMPROF and SIMBAD simulations respectively at a distribution width of 90° and unity sticking coefficient and c) and d) Are simulation outputs from both simulators respectively at a distribution width of 90° and 0.4 sticking coefficient. . 135
Fig 4.5	Illustration of how SIMPROF and SIMBAD simulation outputs in 2D are comparable to each other a) and b) Are SIMPROF and SIMBAD simulations respectively at a distribution width off 135° and 0.2 sticking coefficient and c) and d) Are simulation outputs from both simulators respectively at a distribution width of 180° and 0.4 sticking coefficient. 136
Fig 4.6	Illustration of how SIMPROF and SIMBAD simulation outputs in 3D are comparable to each other a) and b) Are SIMPROF and SIMBAD simulations respectively at a distribution width of 1° and unity sticking coefficient and c) and d) Are simulation outputs from both simulators respectively at a distribution width of 180° and unity sticking coefficient. . . 137
Fig 4.7	Depiction of step and bottom coverage versus deposition widths at unity sticking coefficient. 139
Fig 4.8	Depiction of bottom and step coverages versus deposition widths at sticking coefficient of 0.5. 140
Fig 4.9	Depiction of bottom and step coverages versus sticking coefficients at deposition width of 1° 142
Fig 4.10	Depiction of bottom and step coverages versus sticking coefficients at deposition width of 45° 143

Fig 4.11	Depiction of bottom and step coverages versus sticking coefficients at deposition width of 90°	143
Fig 4.12	Depiction of bottom and step coverages versus sticking coefficients at deposition width of 135°	144
Fig 4.13	Depiction of bottom and step coverages versus sticking coefficients at deposition width of 180°	144
Fig 4.14	Depiction of bottom and step coverages versus deposition widths at unity sticking coefficient.	145
Fig 4.15	Evaporated films a) SEM picture b) Simulation from SIMPROF with constant density c) Simulated film with non-uniform density from SIMPROF and d) Simulated film from SIMBAD	148
Fig 4.16	Sputtered films a) SEM picture b) Simulated film from SIMPROF with constant density c) Simulated film with non-uniform density from SIMPROF and d) Simulated film from SIMBAD.	149
Fig 4.17	Sputtered films a) SEM picture of 8 mTorr b) Simulation from SIMPROF with uniform density c) Simulated film with non-uniform density from SIMPROF and d) Simulated film from SIMBAD.	150
Fig 4.18	Sputtered films a) SEM picture of 14 mTorr b) Simulation from SIMPROF with uniform density c) Simulated film with non-uniform density from SIMPROF and d) Simulated film from SIMBAD.	151
Fig 4.19	a) SEM film of TiW film b) Single SIMBAD simulation showing porous sidewalls. Line segment simulations. Unity sticking coefficient c) Homogenous film density of 1.0 d) Density determined from local sputter flux distribution e) With resputtering model present.	153
Fig 4.20	Experimental and simulated thin films of Titanium on overhang structures a) experimental film b) and c) Simulated films with and without density from SIMPROF and d) Simulated film from SIMBAD. Unity sticking coefficient was used during simulations	156
Fig 4.21	Experimental and simulated thin films of Tungsten on overhang structures	

	a) Experimental film and b) and c) Simulated films with and without density from SIMPROF and d) Simulated film from SIMBAD. Re-emission coefficient of 0.7 is used during these simulations.	157
Fig 4.22	Experimental and simulated thin films of Titanium and Tungsten on overhang structures a) experimental film b) and c) Simulated films with and without density from SIMPROF and d) Simulated film from SIMBAD. Re-emission coefficient of 0.4 is used during these simulations.	158

1.1	Initial topography for vertical wall via/contact structure.	41
1.2	Initial topography for overhang feature.	42
1.3	Deep slanted substrate surface.	42

Chapter 1

1.1 Introduction

Integrated circuits have developed from the invention of transistor in 1947 and evolved into the sophisticated present day technology. Silicon is presently the most important semiconductor in the electronic industry because of a variety of advantages and uses [1].

The first integrated circuit was created in 1960 and since then device densities have increased dramatically. In mid 70's the number of devices fabricated on a chip multiplied to over one hundred thousand devices per chip whereas by 1986 the number was over one million per chip [1]. This shows how fast the number of devices per chip is changing due to the increasing demands of the electronics market. Integrated circuit technology has progressed from small-scale integration (SSI) to very large scale integration (VLSI) and continues to reshape itself. Although the technology is mature at this stage more complexity is being developed [2]. Throughout this development, device sizes have shrunk leading to device miniaturization and the presence of large number of devices on a reasonably sized chip. Device dimensions are shrinking to submicron levels and device density on chip is exponentially increasing with time as shown by Fig 1.1. Device miniaturization has reduced the cost of chips and improved performance.

Fig 1.1 (a) Exponential growth of the number of components per IC chip (b) Exponential decrease of the minimum device dimension

The success of IC technology is partially from the improvement of the processing of thin films. The technology of thin film deposition has made tremendous progress driven by the industrial demand for reliable and robust thin films [3]. That has created strong interaction between the electronic industry and consumers. In addition to major contributions to a variety of technologies, thin film studies have produced research in solid state physics and chemistry in order to better understand the innate characteristics of thin films.

The continued demand for circuits with higher device density has pushed integrated circuit technology to physical and practical limitations. Physical boundaries are set by the classical and quantum limits of electron motion, while practical limitations are from material and lithographic constraints.

A key to success of VLSI design depends on the formation of interconnects between devices. Proper scaling of electronic devices to reduce switching delays and power dissipation requires complex wafer fabrication technologies to ensure their proper operation at higher speeds. Performance of microchip circuits depend not only on intrinsic device performance, but also on the performance of the interconnection of technology.

1.2 Role of metallization in VLSI

The purpose of metallization is to interconnect the various components of integrated circuit. Metallization is an important step for any successful IC design and is achieved through a process of depositing and etching the conducting material to produce metal lines to provide connections to the inputs, outputs and other internal and insulator connections of the active devices in the integrated circuit.[3,4]. During the fabrication process thin metal lines are coated on the surface of the wafer to implement the interconnects. Insulating material is then added, this insulation is then selectively etched (where necessary) to develop more lines and interconnects.

To achieve optimum performance the material selected for metallization should have certain properties to ensure a reliable and effective interconnect. The main points to

issues are:

- Low contact resistance,
- Ease of Fabrication.
- Stability through processing,
- Good corrosion resistance,
- Resistant to electron migration,
- Smooth surface,
- Low stress,
- Conformal coverage throughout topographies,
- Contamination free process
- Low bulk resistivity.

Aluminium is the prime metal used for fabrication of interconnects [1,5]. It has emerged as the main metallic material for such an application because of its low resistivity ($\rho = 2.7 \mu\Omega \text{ cm}$), ease of fabrication and its good adhesion to Silicon and SiO_2 . Unfortunately pure Al has some adverse effects, such as its low melting point (660°C) which prevents its use in certain applications. The limitations of pure Al that restrict its use in VLSI are partially overcome by using Al alloys [6]. These alloys have shown a better resistance to electron migration specially at higher temperatures. Typical alloys are Aluminium-Silicon and Aluminium-Silicon-Copper alloys. Since there is no material that satisfies all

the requirements for an interconnect technology, it is a matter of judicious choice to select the appropriate material suitable for a specific application.

1.3 Multilevel Metallization

The decreasing feature size of devices to sub-micron levels and to sub-quarter-micron in the future is driven by a desire for high device densities. In order to achieve high density circuits the interconnect structure becomes very complex. Multilevel metallization is the only solution to fabricate these structures and to maximize chip area utilisation[7,8].

To form a multilevel metal structure metal lines are isolated from each other by dielectrics layers. The dielectric layers are patterned and etched to form vertical connections (vias) between metal layers. Patterning, etching, and deposition of dielectric and metal layers are carried out as much as required to fabricate a single device or an IC with a complete metallization scheme [8].

To minimize intermetallic reactions and improve reliability, metals like tungsten are sandwiched between the metal layers to improve the characteristics of contacts and raise the resistance of aluminium diffusion to the silicon (reduce junction spiking) which is a key factor of VLSI design failure. Silicides are often used for contacts to enhance the required electrical properties of the contact [9]. As a final step of VLSI or ULSI design implementation, the chip is passivated, bonded and packaged.

A critical part of multilevel metallization is the deposition of metal layers with good thin

film properties. Fig 1.2 is half cut view of single device showing all major parts of the device processing including metallization.

Fig 1.2 A cross-sectional view of a single MOS device illustrating two level metallization process.

1.4 Deposition methods

Deposition of thin films of semiconductors, metal alloys, and photosensitive materials are

indispensable for the fabrication and production of integrated circuits and related devices. Although the intrinsic material bulk or surface properties can not be influenced, the deposition techniques can be optimized to attain the best use of material properties.

To properly select the appropriate deposition technique a number of issues should be considered:

- Suitability of film material.
- Deposition technique (chemical, physical, selective or nonselective).
- Deposition rate and deposition environment.
- Film coverage over topography.
- Equipment maintenance and cost.
- Final cost per unit produced.

There are three basic steps to form a deposition of thin films by vapour techniques over the desired substrates and they are:

- Creation of the vapour species to be deposited.
- Transport of these species from the source to the substrate.
- The deposition of the transported species on the substrate.

If there is no chemical reaction involved in any of the steps, the deposition technique is termed as physical vapour deposition (PVD), otherwise the deposition is classified as

chemical vapour deposition (CVD). Common deposition techniques can be divided into three types:

- Thermal evaporation (physical vapour deposition).
- Cathodic sputtering (CS) and
- Chemical vapour deposition (CVD).

1.4.1 Thermal evaporation

When solid material is heated to a sufficiently high temperature it melts and evaporates. The evaporated material is then transported via diffusion to the cooler substrate where it condenses[10]. There are several ways to generate a vapour source such as resistive heating, inductive heating (RF heating) and electron beam evaporation.

Resistive heating was the method of choice in the past but is not used as much today. Normally twisted coils made of refractory metals are wound over a crucible that is made of either oxides, graphite, pyrolytic or refractory metals. The crucible is then heated by passing a current through the coil [10, 11, 12]. Induction heating uses thin crucibles and a RF field to melt and vaporise the material. Resistive heating is rarely used because, a) The metal to be evaporated melts and wets the filament material of the heater, and b) refractory metals can not be evaporated because of their high melting point and the fact that the filaments themselves are made of refractory elements.

The electron-beam method uses a directed high energy beam of electrons to heat the

material which eliminates problems of wetting while yielding a highly pure film on the substrates. A Tungsten filament is heated to supply electrons which are accelerated by a positive potential applied between filament and the material targeted for evaporation. The energetic electrons lose their energy in the material by collision and the surface of the material melts and evaporates. Magnetic fields are used to control the electron optics so heating and material evaporation occur at selected surface locations.

1.4.2 Chemical vapour deposition

A chemical vapour deposition (CVD) is defined as a method in which the desired constituents in the vapour phase react on the substrate to form a solid film [10]. A major advantage of chemical vapour deposition relative to other methods of thin film deposition is the high degree of conformal coverage it can produce [13]. CVD process offers the following advantages [1]:

- Highly pure deposits are easily achievable.
- Different materials of different chemical compositions can be deposited.
- Cost effectiveness and control flexibility are possible and
- Some films cannot be deposited with adequate film properties by any other method.

However the structure of material deposited is limited by the existence of an appropriate surface reaction. Deposition of dielectrics and polysilicon layers over substrates by using CVD have been in use for a long time. This method for metallization is common for

Tungsten plug technologies.

Most chemical vapour depositions operate at high pressures and consequently the species from the source have a small mean free path (λ) which is defined as the statistically random distance travelled by vapour atoms or molecules between successive collisions.

The distance between successive collisions can be calculated as

$$\lambda = \frac{kT}{p\pi\sigma\sqrt{2}} \quad [7]$$

where k , T , p and σ are Boltzmanns constant, temperature, pressure and molecular diameter respectively. The small mean free path (mfp) results from a collision process during the transport of species to the wafer.

1.4.3 Sputtering processes

Sputtering is the mechanism of directing charged particles (usually ions) to the surface of a material to dislodge atoms from it. Atoms are ejected from the target and then transported through a low pressure chamber to the surface of the substrate where they condense to form the required film. There are two standard ways to create energetic ions for sputtering to initiate the process, DC diode sputtering and radio-frequency sputtering (RF sputtering) [1]. Sputtering is very suitable for VLSI depositions, and is the most common method of depositing metal thin films.

Sputtering is a kind of physical vapour deposition and is a widely used technique for many different kinds of metallic depositions [4,8]. During sputtering a stream of ions are directed to the target surface and when the ion reaches the target the following actions can take place:

- The ion can be reflected being neutralized through the process.
- The impact of the ion on the target may knock out an electron, known as a secondary electron, from the target surface.
- The ion may be buried in the target resulting in what is known as an ion implantation.
- The ion impact can create structural reformation that could range from simple vacancies and interstitial sites to gross lattice defects and radiation damage.
- Ion bombardment can eject atoms from the target surface and this is known as sputtering.

In a sputtering system most often a plasma is formed below the target as a source of ions and a large negative DC or RF potential is applied to the target of the sputtering system. This potential attracts ions from the plasma and accelerates them into the target where they knock-out atoms from the surface of the target. In both DC and RF sputtering, most secondary electrons emitted from the target do not cause the required ionization events in the plasma. They end up being collected by the anode substrate where they cause unwanted heating. Both DC and RF sputtering also exhibit inadequately low deposition

rates. To raise the efficiency of the system, magnetron sputtering is used, in which magnets are placed at the back of the target to confine the accelerated electrons in the plasma to the region of the target and to increase the percentage of ionization.

During transport, collision occurs between the sputtered material and the inert gas in the sputter chamber. This causes the sputtered material to scatter in all directions depending on the energy of the sputtered species and the pressure of the sputtering chamber. The mean free path of sputter system is large compared to that of CVD, since it operates at low pressure. Therefore, many species striking the substrate are unscattered and can have significant energies.

1.4.3.1 Bias sputtering

A variation on sputtering is bias sputtering: During bias sputtering a negative voltage is applied to the substrate holder while the rest of the system remains as before. Under this condition energetic ions will strike the substrate and the wafers are being coated and etched simultaneously. The deposition rate of the growing film is controlled by the substrate bias. Resputtering film material is very useful in controlling the properties of the deposited film by redistributing the film.

Bias sputtering has been found effective to alter a broad range of properties of deposited films such as resistivity, step coverage, grain size, surface roughness, density and etch rate [11]. The amount of the material that is re-sputtered is roughly proportional to the

negative bias of the substrate and the deposited film is re-sputtered as fast as the ions arrive to the substrate [14].

1.4.3.2 Directed sputtering

Magnetron sputtering is widely used to deposit metal layers on semiconductor wafers. However, This deposition process is inappropriate to deposit conformal films into deep structures as the line widths decrease and aspect ratios of the topography increases [15]. The main problem of standard magnetron sputtering is its inability to deposit enough film at the bottom of a deep surface structure. A number of sputtering techniques have been developed to improve bottom and sidewall coverage of the deposited film such as barrier layers.

The dominant reason for the poor bottom coverage using the standard system is the wide angular distribution of the depositing flux at the substrate. A wide angular distribution of flux results in a significant amount of shadowing that reduces substantially the deposition rate at the bottom of the feature. This wide angular distribution is due to a small target/substrate spacing and the working high pressure that produces significant gas scattering, see Fig 1.3 part a). A common modification of the standard sputtering system to improve bottom coverage can be either by using a collimator or using long throw sputtering [16,17] (see Fig 1.3b and c).

For the arrangement which uses a collimator, a physical filter is inserted between the

Fig 1.3 Schematic depiction of a) Standard sputtering system b) Long throw sputtering system and c) Collimated sputtering system.

target and the substrate. This filter consists of a periodic lattice of holes which filters out the oblique adatom flux to the narrow angular distribution of the flux striking the wafer [17]. The effectiveness of the system is primarily determined by the geometry of the collimator and its position in the system. The second arrangement is long throw sputtering, which takes advantage of sputtering technologies that allow for very low working pressures that reduce the working pressure to less than 0.5 mTorr. At these pressures the substrate/target distance can be greatly increased without appreciable gas scattering

being, see Fig 1.3 part b). The angular distribution of such a system is determined by the geometry of the system.

The primary goal of long throw and collimated sputtering is the narrowing of the angular flux at the substrate and the production of a direct flux perpendicular to the wafer. The performance of these systems are determined by the geometry of the system and the operating pressure, target/substrate spacing, target size and erosion profile. At moderate pressures (2- 10 mTorr) the angle of distribution is strongly dependent on the mass of the sputtered species. At these pressures, an average sputtered atom will undergo only a few collisions, and the heavier atom forward momentum will persist for a large number of collisions resulting in a narrower distribution [17]. In traditional sputtering the use of working pressures in the region of 2 mTorr produces typical mean free paths of order of 1 cm. Typical target to substrate spacing are around 3- 10 cm and particle fluxes arriving at the substrate are generally below a few electron volts. At pressures below 1 mTorr the mean free path is of the order of 10- 100 cm and fluxes striking the surface have undergone very little scattering. The effect of lowering the pressure substantially improves bottom coverage due to a narrowing angular distribution of the depositing flux. But there is also a possibility of re-emission that can enhance sidewall coverage.

1.5 Thin film properties

While a multitude of film properties may be considered, the most important ones for VLSI design are as listed in Section 1.1 above. Although the properties of a bulk material

may be well characterized, the same material in a thin film form may have a substantially different properties from those of the bulk. The reason is that, thin film properties are strongly influenced by surface properties and microstructure, and in 2D along the surface where as the bulk materials characteristics are determined by its 3D structure. A thin film, by definition has a substantially higher surface-to-volume ratio than does a bulk material. The structure of thin films, and their method of preparation also plays a vital role in determining film properties.

Many properties of thin films depend on the choice of the deposition technique as well as on film properties. Film structure is strongly determined by deposition method. Thin films are usually made of many tiny grains separated by grain boundaries. If the separation exceeds certain critical value, voids could emerge in the grain structure and can lead to a phase transition from conducting to non-conducting films [1]. In technology of thin films, it is necessary to have high density of the deposited material and to have very low density of all kinds of particulate defects to ensure proper operation.

1.6 Growth mechanics

Atoms from the vapour phase are condensed to a solid on a substrate by the interaction of impinging atoms with the surface of the substrate material [10]. Impinging vapour molecules can be either adsorbed and permanently fixed to the substrate, adsorb and evaporate in a finite time or they can immediately reflect off of the substrate [8,10,14].

As the impinging atom reaches the surface of the wafer, attractive forces make it adhere

to the surface and an adatom is formed. For the vapour atom to be attached to the surface, it must transfer its normal component of velocity to the surface [18,19]. When that velocity is transferred, attachment of the vapour atom follows. If the atom is only attached to the surface loosely it is known as physisorption. If the atom links strongly with the surface using chemical bonds the process is called chemisorption. Adsorbed atoms may continue to move along the surface (moving from one potential well to another) according to the kinetic energy associated with them, their initial lateral velocity and the thermal energy of the surface. In some cases, re-evaporation of adatom may take place.

1.7 Nucleation and growth

During the first stage of growth the adatoms move along the substrate surface eventually combining with other adatoms on the surface to initiate nucleation. If the adatoms form a cluster with radius greater than the critical size, their free energy decreases with the increasing size, thus favouring growth to continue [1,10,20]. If on other hand the cluster radius is less than a critical radius, then the clusters disintegrates and starts to re-evaporate, producing no net growth. Whenever a new critical size nuclei is formed, a new island is started.

With the aid of electron microscopy several stages of growth have been observed. The island growth stage occurs when growth parallel to the surface of the substrate is larger than growth normal to the substrate. This stage is followed by a coalescence stage where

different nuclei contact each other and form larger shapes. This effect arises as the result of diffusion of adatoms along the surface. The total exposed area of the substrate is reduced at this stage [1]. Larger islands are created and continue to grow leaving behind channels or holes. Again, the channels are filled by secondary nucleation, to create a continuous film and growth continues as long as there is an adatom supply.

1.8 Film structure

The term, film micro-structure, encompasses a variety of concepts which describe the internal arrangement of the thin film. The determination of the material structure of thin films depends on shape of the topography deposited over, the substrate temperature, deposition technique, type of the material and ambient pressure under which the deposition was carried out [21].

The microstructure of a thin film is in part determined by the orientation of the film flux deposited on the substrate, and is therefore a function of local topography. A description of thin film microstructure developed by Movchan, Denchishin and Thornton [16] charts the transition from a highly porous columnar film (Zone 1) at low substrate temperature, to a dense columnar grain structure (Zone 2) at elevated substrate temperature and then to a recrystallized dense grain structure (Zone 3) at very high substrate temperature. This transition occurs as the adatom energy is raised, either by raising the relative substrate temperature or by lowering the working pressure. All sputtered refractory metals exhibit Zone 1 characteristics while aluminium and copper have Zone 2 characteristics when

deposited at room temperature.

Higher substrate temperatures and lower deposition rates tend to create very large grains, while lower substrate temperatures and higher deposition rates create amorphous deposition. Conditions at an intermediate level have tendency to create polycrystalline films. Surface roughness is also a function of temperature and depositions at higher temperatures tend to be smoother. This is due to a higher mobility of adatom species which fills peaks and the valleys of the structure. Higher temperatures may, however, have an adverse effect due to faceting which can increase surface roughness.

Another important factor is the density of a thin film which gives information of its mass-volume relationship. If the density is low it shows that the grown film is porous, and its material properties may be severely degraded.

1.9 Electrical properties of thin films

The basic electrical requirement of a thin metallic film is a low resistivity and the capability of handling reasonably high current densities. A low resistivity is particularly important in order to assure minimal power dissipation and small propagation delay in the interconnects along the runs. Delay is directly proportional to film resistivity, square of line length and inversely proportional to film thickness. Thicker films and shorter lines should be used whenever and wherever it is possible to further minimize resistivity and delay [22].

High temperature deposits show the lowest sheet resistivity due to a large grain size, lower defect and impurities while lower temperature deposits show the highest resistivity [14]. The sources of such resistivity are from extrinsic impurities, vacancies, interstitial atoms, dislocations, stacking faults and the nature of the deposited material etc [1]

A good, low resistance contact is needed between the metal and semiconductor and is usually formed by depositing metal or silicide on the semiconductor. A metal is then deposited over the contact to give a low resistance path that is necessary for the conduction of current [7,14]. A good contact should not disturb the device characteristics and should be stable electrically and mechanically. The total resistance of the contact is comprised of two components in series, the semiconductor bulk resistance beneath the contact and the resistance of the metal semiconductor interface [5].

1.10 Contacts and vias

When a device is created in a silicon wafer, a contact has to be made down to the device to allow a passage for the current [23,24]. A contact or a via is a cut in the dielectric layer which is used to interconnect two layers of conductors, whether an active region or a layer of metal. A via is a metal to metal interconnect while a contact is a metal to semiconductor interconnect. To form a contact an oxide is coated over the substrate surface. Windows are then opened in this oxide by using wet or dry etching techniques.

Once the window is opened in the interlevel oxide insulator, metal is deposited over the holes to form a connection between the two conductive layers. As design requirements

move toward reduced feature sizes, well below $1\mu\text{m}$, significant problems emerge in via fabrication technology and fabrication constraints put special demands on metallization schemes. High aspect ratios of contacts/vias in submicron VLSI designs can cause reliability problems. The height to width ratio of a via or a hole is called its aspect ratio. Poor film coverage can result in reliability problems such as open circuits with corresponding device failure [25].

1.11 Barrier and encapsulation layers

Contact and interconnect barrier metallization present well recognized problems in VLSI technology. The problem of contact stability arises from two phenomena: contact thermomigration and contact electromigration. Thermomigration, which often is referred to as spiking, is a process of mass transport across the interface that takes place in the absence of an applied bias, and results a deep metal penetration into the junction [23,24]. The high Si solubility in Al allows Si to move into Al and Al to move into the substrate to replace the displaced Si. Another kind of failure is electromigration which is a transport of metal atoms under conditions of high current density. Bilayer and trilayer contact structures formed out of a variety of materials are used for VLSI interconnections [26]. These structures provide good adhesion and also serve as a diffusion barrier to Al.

To form a bilayer structure a material that can provide the necessary adhesion to Silicon surface and also can serve as diffusion barrier is deposited over silicon substrate surface followed by an interconnecting conductor such as Al 1% Si. As there is no unique VLSI

metallization scheme, a unique barrier layer does not exist, but cost effective solutions for barrier deposition continue to be developed and implemented [25]. An example of a trilayer structure is Titanium to provide good adhesion to Silicon and TiN layer as a diffusion barrier and Al as the interconnecting material. A typical structure is shown by Fig 1.4.

The wide spread use of aluminium and its alloys as contact and interconnect metallization, stems from some major advantages it offers, but it is susceptible to junction spiking at high temperatures and has poor electromigration resistance. To prevent this problems, an option to deposit three-layer-metal sandwich [26] was proposed as shown by Fig 1.4. In this method, a thin layer of aluminium is separated from its bulk conductor by a metal conductor, such as tungsten, that acts as a diffusion barrier. The thin layer of aluminium that is deposited first is sufficient to provide good ohmic contact and good adherence characteristics, but is insufficient to cause spiking failure because of its smaller quantity. Other studies concentrate on bilayer barrier systems; using titanium as a barrier agent. Upon sintering, Ti slowly reacts with Al to form an intermetallic compound. The action of Ti as a barrier continues only as long as Ti is still present to feed the reaction. If all the Ti is consumed, then Al attacks the silicon substrate and spiking may start. Development of a suitable barrier will depend on the availability of data of interdiffusion and growth kinetics of compounds in multilayered films.

Fig 1.4 Via and contact schemes

Al and its alloys have been extensively used as a wiring material for Si devices. However their electrical resistivity and reliability will limit the use of this material in deep submicron devices [27]. Copper has been suggested as a possible substitute for Al alloys in VLSI technology because of its higher conductivity and its potentially greater resistance to electromigration [28]. However, copper diffuses in to SiO_2 and Si substrates during device fabrication and operation. Therefore, a barrier layer to prevent Cu diffusion must be used.

Tantalum and Tantalum alloys are among the promising candidates for ultra thin metallic diffusion barrier and adhesion layer applications in copper based interconnects [29]. Ta is

deposited on all areas where copper can diffuse and copper is deposited afterwards. Ta is again deposited on top of the copper to complete the encapsulation. This creates the encapsulated layer of copper which prevents copper diffusion as shown in Fig 1.5.

Fig 1.5 Encapsulation schemes.

1.12 Step coverage and bottom coverage

Poor film coverage is one of the most serious problems in realizing submicron multilevel interconnections. The most difficult steps to cover are those with straight walled topographies [14,20]. Step coverage is measured as how well the deposited film covers the side walls of the via or contact. It is defined in different ways by different people and there is no consistent way of expressing it. We shall define it as following. A is the minimum thickness of deposited material along the side wall and B is the nominal thickness of the film on flat regions of the via as shown by Fig 1.6a and step coverage is given by the

relation $A/B \times 100$.

Aspect-ratio is defined as the height-to-spacing ratio of two adjacent steps of via (height/width) as shown by Fig 1.6b. The greater the step height (greater aspect ratio) the more difficult it is to get conformal coverage. In recent years the aspect ratio has been increasing with each new technology because W shrinks as device size shrinks but the dielectric thickness remains almost constant.

Fig 1.6 a) Depiction of step coverage of via and b) Depiction of aspect ratio of

Angular distribution of the incident flux striking the wafer is a major factor in determining step coverage. With a sharp vertical angular distribution, 1° or less, the top and bottom surfaces of vias or trenches receive the maximum possible coverage, but there is almost no step coverage. As the angular distribution increases, step coverage improves, because the vertical surface is exposed to more flux. However, step coverage is only

improved at the expense of the bottom coverage, since there will be less flux at the bottom surface due to shadowing of the large angular distributions. Bottom coverage is also affected by the self shadowing of the growing film itself, and that could cause severe problems at bottom corners.

1.13 Topography of vias and contacts

Via topography is important in determining a number of important factors. Straight side-walled vias require less effective area, than those with sloped side walls and are desirable for high device densities. However, steep side walls (straight walled vias) give rise to step coverage problems, because of the metal thinning at the bottom corners of these steps which can even cause discontinuity as shown by Fig 1.7a. Since vertical profiles present difficulties with respect to the uniformity of step coverage, tapered topographies which could significantly improve step coverage can be used as shown by Fig 1.7b. If sloped vias are used, the minimum area of the vias would be larger than if vertical ones are used affecting device density.

Fig 1.7 a) Metal discontinuity caused by steep via hole because of shadowing effect and b) Improved step coverage using a tapered profile.

Stacked and staggered types of vias are extensively used in advanced processing of multi-level metallization. Metal 1 and metal 2 of stacked vias are located on top of silicon or polysilicon contacts and on the top each other. Such a type of via may result in steep topography and step coverage problems may arise if sloped vias are not used [8,24]. Fig 1.8 shows the profile of a stacked via.

On other hand, in staggered vias the connections from metal2 to the silicon are done through a metal-1/silicon contact. If sloped vias are used, then metal patterns must be wide enough to prevent etching of grooves on the side walls when deep vias are being opened [24]. A Staggered via scheme provides an adequate step coverage, but it can result in a large chip size. Fig 1.9 shows a contact scheme of a staggered via.

Fig 1.8 Contact scheme of stacked via.

1.14 Simulators

Process simulation is the physical modelling of process steps with the aid of a computer using formulated mathematical models to describe the physical phenomena. If the resulted simulation resembles the experimental results, the obtained simulation output is considered to be sufficiently reliable.

Device design has become so complicated that it would be prohibitively expensive to optimize process sequences using only experimental techniques and that has resulted in simulators being used extensively [30,31]. Simulators are becoming more popular as the

Fig 1.9 Contact scheme of staggered vias

cost of performing an experiment rises and the cost of computation decreases from year to year. As a result computer simulations are regarded as a useful tool to predict actual process sequences, while the actual experiment establishes the validity of the simulated model. However, during simulation small errors in each individual step can accumulate and the final predicted profile may be in considerable error. Despite their limitations, simulators can provide reasonably accurate quantitative result when used appropriately.

In the course of semiconductor process simulation selected sequences of simulating steps are carried out. There are two main types of process simulators; front end (doping profiles and oxide growth) and back end (metal and oxide deposition and etching). Front end simulation is mature, but back end simulation is still in its infancy. During the simulation of the deposition of thin films, a back end process simulator has to account for two

things; transport of the adatom flux from the source and the topographical evolution of the device features.

By using simulators it is possible to analyse deposition characteristics and properties [18]. In advanced metallization processes, requirements that are to be exhibited by simulators are a) cost effective, b) fast, c) capability to simulate variety of deposition techniques, d) ability to represent submicron topographies, e) ease of use, and f) close correspondence between simulated and actual processes.

To develop a simulator, theoretical approaches for explaining physical problems and the rules for the phenomena under consideration are investigated to understand it thoroughly. Analytical formulations are then developed to solve physical quantities at hand, rigorously or by means of approximation. Algorithms to implement physical calculations are then arranged and the code to perform a computer simulation is created.

Engineering workstations are used to do these kind of simulations and their speed is a function of workstation capability and the simulator's algorithm. In general, simulators are intended for use in production facilities. Simulators are also widely used in educational institutions.

1.15 Types of models

There are several approaches to simulate thin film growth to model the necessary evolution of a growing surface. Four basic types of simulators have been developed.

- 1) Molecular dynamics
- 2) Atomistic Monte Carlo model
- 3) String algorithm model and
- 4) Ballistic models

Types 1 and 2 account for interaction and positions of individual atoms, while 3 and 4 are concerned the macroscopic growth of the film. Each of these models will be described in the next four sub-sections.

1.15.1 Molecular Dynamics

Molecular Dynamics (MD) models explicitly all the atoms in the region of the substrate. Each atom is modelled using classical physics and an inter-atomic potential. In order to carry out MD simulations, a detailed understanding of complex kinetic processes is necessary [32,33,34]. The forces between all combinations of interacting atoms are computed and the classical equations for all particles are solved simultaneously and their trajectories are followed throughout the simulation [35]. Huge numbers of atoms are involved in such a detailed analysis of atomic interaction and very detailed data is acquired which is of potentially great use. Unfortunately, since the position, energy and velocity of each of these atoms is required for each time step, Molecular Dynamics simulation require an extremely large computational effort.

The enormous calculations involved and the necessary memory requires super-computers to carry out such a simulation[32]. These enormous computational requirements seriously limit the application of MD simulations as process development tool [18]. MD is therefore an unacceptable model for direct process simulation of practical devices due to computational limitations[35].

1.15.2 Atomistic Monte Carlo Model

Atomistic Monte Carlo (MC) simulations also deal with individual atoms in the simulation region. However, the physical models used to describe the atoms behaviour are not derived from detailed atomic interactions, but a stochastic approach is used. The average atomic movements are modelled using either laws from statistical mechanics or empirical relationships. Monte Carlo techniques are therefore significantly more efficient in calculating the movements of the atoms. However, the large number of atoms present in $1\mu m \times 1\mu m \times 1\mu m$ region of solid is still prohibitively large and computationally extensive so that the method is limited in its applicability to full process simulation. Approximations to the calculations have been used in atomistic MC simulation to increase the number of particles simulated, and detailed micro structure information can be predicted. However, MC is not applicable to integrated circuit processes due to its complexity [18].

1.15.3 String algorithm

Macroscopic process simulation of IC technology is often used to rapidly and economi-

cally explore process steps and effects. Several computer programs based on segment motion have been developed to model thin film deposition processes [37]. This type of simulation represents the film surface as a series of a short segments that constitute the whole topography. String models compute flux components reaching the surface profile while accounting for shadowing effects and surface diffusion. During these calculations the centre point of each segment on the surface is considered as the flux receiving point.

These models are very practical and can easily be implemented on present day workstations. Unfortunately, string algorithms can not represent the internal information needed to depict microstructure. During a simulation, line segments are advanced serially one after another up across the topography, and a new layer of the film is grown. This is continued until the desired film is grown. String algorithms are simple and fast and have attracted significant interest. The accuracy of the model and its applicability to IC processing is tested by comparing the simulated profile output to the experimental results.

1.15.4 Ballistic deposition

Ballistic deposition models are not very different than Atomistic MC models except that they use aggregate discs rather than atomistic data structures to simulate etching or deposition over vias and trenches [18,38,39]. The trajectory of each disc represents a large number of atoms that move through similar trajectories. Modelling the growth of a thin film using ballistic aggregation provides information regarding the microstructure of the film. This model also simulates the film deposition over topography, but is computer

intensive with regard to both execution time and memory. In the model, particles (either circles of unit radius in 2-D simulations or spheres of unit radius in 3-D simulations) are deposited at on substrate topography by using stochastic processes [40]. This kind of simulation was first developed for diffusion limited aggregation and related growth processes and then evolved toward topography simulation for thin film growth.

Modelling of thin film microstructure is becoming important as the microelectronic devices are further miniaturized [41]. Ballistic deposition modelling is becoming extensively popular because of its successful prediction of columnar growth and structure profiles [42]. A ballistic deposition program, SIMBAD, will be briefly discussed in Chapter 4.

1.16 Motivation for SIMPROF

The purpose of this thesis is to describe and report the development of SIMPROF (a line segment simulation for topography evolution). The main goal is to develop a model that can produce reliable output in a reasonable span of computational time (less than 1 hour) by using string algorithm.

This program has been developed to simulate thin film coverage over vias and trenches by calculating the incident and reflected fluxes and subsequent deposition. A primary motivation of the project was the development of an alternative simulation frame work for the Carleton University and University of Alberta thin film simulation group. The group has developed a sophisticated set of programs known as SIMBAD. SIMBAD is a

deposition and etching simulator based on a discrete data base and Monte Carlo algorithm. The main difference between SIMPROF and SIMBAD is the use of a string algorithm by SIMPROF to update its surface evolution, whereas SIMBAD uses ballistically aggregated discs, in which each disc represents the final resting place of a large number of atoms. An example of SIMPROF's simulation output is as shown by Fig 1.10(a) and Fig 1.10(b) shows a SIMBAD counterpart.

A number of advantages are present for different types of simulators. Chiefly for SIMPROF the major advantage is the relative ease with which a nodal based data structure can be used for a discrete version of the diffusion equation used to describe the surface physics and flux transport. The main disadvantage is the complications that arise in surface movement.

A strong motivation for the development of SIMPROF was to enable comparison with SIMBAD simulations. Situations sometimes appear when algorithmic problems are difficult to separate from physical effects and two differently based simulations can be used as a tool for investigation.

Fig 1.10 a) Simulation output from SIMPROF and b) Simulation output from SIMBAD over a trench with a thickness of $1\mu\text{m}$ and distribution width of 1^0 .

Chapter 2

2.1 An outline of SIMPROF

SIMPROF (Simulation Profile) is a line segment topography simulator written in the C language. It needs as input the initial topography, incident flux, an adatom flux angular distribution for the incident flux and run parameters. It is specifically designed to simulate 2D and cylindrically symmetrical quasi-3D surfaces to provide the energy and the angular distribution of the sputtered flux [43,44]. A three dimensional Monte Carlo simulator SIMSPUD (simulation of sputter distributions) that simulates vapour flux transport is used. The angular distribution from SIMSPUD is then passed to SIMPROF. If data from SIMSPUD is not used a variable width cosine distribution can be used.

When performing a simulation the first step is to compute the incident flux striking the surface. In order to determine the flux striking all segments on the surface of the substrate, SIMPROF has to calculate the magnitude of the flux reaching each segment on the substrate. The program considers whether the flux incident to the profile partially or entirely sticks to the surface. In the course of the calculation SIMPROF has to consider the incident flux distribution from all sources (from the top of the simulation region or reflected from the substrate topography itself), the geometry of the substrate and the topography of each node and segment. Visibility is very important and SIMPROF needs to determine if the incident and reflected fluxes are shadowed by other segments.

This simulator also considers the effects of surface diffusion, different growth

algorithms, surface looping and the variation of thin film density on the substrate surface. It also has the ability to model diffusive, chemical, specular and resputtering flux re-emission mechanisms.

The flow charts in Fig 2.1 and Fig 2.2 (2D and quasi 3D respectively) illustrate the basic execution of the program. The difference between the 2D and 3D flow charts arises from the simulation of reflection phenomena. For 2D simulation both reflective and non reflective species of flux are dealt with while 3D deals with only incident flux. After initialization the program parses through the input commands and sets parameters. Once the input parameters of the program are set, SIMPROF starts executing the process simulation. During execution several different computations are performed to implement the thin film simulation processes. Throughout the process the program calculates the incident and reflected fluxes applying the necessary visibility tests. It then computes the adatom diffusion and determines the amount of material to be adsorbed on the surface. As the growth rate is now fully specified the surface is advanced and data structures are updated. If the required film thickness is not yet grown, the process continues to run until the required thickness of the film is grown. Throughout the process a number of issues such as source representation, visibility, flux calculations, flux distribution, adatom diffusion and flux data structures have to be dealt with and these will be described in detail in this chapter.

Fig 2.1 Flow chart for 2D simulation model.

Fig 2.2 Flow chart for 3D simulation model.

2.2 Initial surface representation

Before initiation of any simulation the starting substrate topography of the via or hole has to be defined and created. The dimensions of the surface topography are defined in a file. Special routines are then used to read the information from that file and store it in a data structure. The initial topography is a set of segments from which the substrate topography is constructed by the program. The size and the shape of the topography can be easily altered just by editing the initial file to get any profile of your choice. Each of the following tables specifies one substrate configuration as shown by Fig 2.3a, Fig 2.3b and Fig 2.3c

1.1 Initial topography for vertical wall via/contact structure.

Table 1.1

0	3	3	1.0
0	2	-99	
0.9	2	-99	
0.9	0.5	-99	
2.1	0.5	-99	
2.1	2	-99	
3	2	-99	

1.2 Initial topography for overhang feature.

Table 1.2

0	3	5	1.0
0	2	-99	
1.8	2	-99	
1.2	1.5	-99	
0.4	1.5	-99	
0.4	0.5	-99	
2.6	0.5	-99	
2.6	1.5	-99	
1.8	1.5	-99	
2.4	2	-99	
3	2	-99	

1.3 Deep slanted substrate surface.

Table 1.3

0	2.0	3.5	1.0
0	2.8	-99	
0.5	2.8	-99	
0.48	2.7	-99	
0.6	0.3	-99	
0.65	0.20	-99	
1.0	0.15	- 99	
1.35	0.20	-99	
1.4	0.3	-99	
1.52	2.7	-99	
1.5	2.8	-99	
2.0	2.8	-99

Fig 2.3 a) Surface created from Table 1.1 definition of topography b) Surface created from Table 1.2 definition of topography and c) Surface created from Table 1.3 definition of topography.

The first line of each file describes the maximum x and y dimensions of the topography. The next n lines are n points describing the substrate geometry. Each line contains an x and y position and a series of numbers indicating the substrate point location. The number -99 is a compatibility factor with SIMBAD.

2.3 Surface data structures

In SIMPROF The physical surface is represented as a linked list of segments. Each segment/node is represented by a data structure. The surface data structure is organized into blocks of memory locations which are linked together. Each block contains one pointer to the next block, so they form a chain, and the entire collection of linked blocks is called a linked list. However, the structure of this type is unidirectional, and we will need to have bidirectional activity through the list.

To reach our intention of going in any direction through the linked information stored in each specific block, we simply extend the linear list by supplying two pointers to each block of memory. One of the pointers points to its successor (next block or node) and the other to its predecessor (previous block or node). This creates a data structure of double linked lists which is sufficient for our purpose. The physical surface of the substrate is represented by series of linear segments. The necessary information of surface physical data and geometry over which the thin film is to be grown is stored in the surface data structures as Fig 2.4 shows. Each node on the surface can access the information it requires from specific blocks in the data structures.

To update the surface of the evolving topography the stored information is deleted once a layer of thin film is grown and new data for the next layer has to be calculated right after deletion. The newly obtained necessary data is then stored in the data structure to prepare for the next layer of growth. This trend continues until the anticipated thickness of film is grown. Throughout the data structures two surfaces (previous and

next) are available.

Fig 2.4 Depiction of data structure arrangement.

2.4 Incident flux source representation in SIMPROF (2D and 3D)

In every simulation there must be an adatom source to supply the necessary material to be deposited over the topography. In SIMPROF there are two types of sources

line and plane sources at the top of the simulation region used by two dimensional and three dimensional simulations respectively. For 2D simulation the line source is divided into many individual sources (m segments) to approximate the flux from the top of simulation region.

For 2D source line we consider the matter emanating from each source segment stepping through the source line until all the flux from the line source is accounted for. In this way we account for the amount of flux gathered by one segment of the film surface from each segment on the source line as shown by Fig 2.5. The amount of incident flux to each segment (node) of the substrate is the summation of all the fluxes arriving it from the total length of the source.

Fig 2.5 Flux contribution from source line to specific

For the case of a three dimensional (3D) simulation, the source points are far more numerous than its two dimensional counterpart as it uses a plane source rather than a line. In this case the whole top surface of the simulation is divided into small areas that make up the flux source. Each of these areas is examined strictly and carefully and the amount of incident flux from it is assessed and added to the beneficiary node. To devise a systematic way of evaluating the incident flux from different source points on the plane,

the source is constructed as a circle having a centre coincident with the centre of the via or topography. The radius of this circle is half of the line source length and is located at a height above the surface profile. We subdivide the source into smaller parts to facilitate flux simulation. The diameter(D) of the circle is then divided into m parts of $\Delta L = D/m$ length each, as we did in two dimensional case (line source). Another circle which is concentric to the constructed one is created. This new circle has a radius (r_2) which is one step of ΔL length less than (r_1) of the constructed circle, where both r_1 and r_2 are at π radians as shown by Fig 2.6. Then we fix $\Delta\theta$ which is equal to π/n where n and m can have any value but are normally set to around 100.

After designating that values (r_1 , r_2 , ΔL and $\Delta\theta$) r_1 and r_2 are rotated from 0 to π radians by an angle $\Delta\theta$ radian at a time. The area of each sector subtended between r_1 and r_2 before and after they were rotated is as shown by Fig 2.6. The area of this minute sector is proportional to the magnitude of the mass moving from that sector to the substrate. To add up all the flux from the source to one segment we iterate the above process m times in L loops over the entire source surface estimating each time the amount of flux received by specific substrate segment.

At this point we have calculated only the amount of material from the half of the constructed circle toward a single segment on the surface and it is necessary to get the flux from the other half. Fortunately, since the two halves of the circle are symmetrical we only double the magnitude from the former half and all the material from the source is accounted. The total number of incident points (T) to single segment on the surface in

three dimensional case is $T = l \times m$ where l is the number of sectors in a loop and m is the number of divisions in diameter.

Fig 2.6 Flux contribution from plane source to specific substrate segment: we only considered one loop of the plane source for simplicity.

2.5 Incident flux Distribution

Before we proceed to calculate incident flux to the surface we need to define the flux angular distribution from the source. The flux distribution from a line or plane source can be represented by a user defined cosine distribution or an output file from the SIMSPUD transport model. The SIMSPUD model will, given the geometry and sputtering conditions, provide the distribution of the sputtered atoms arriving at the substrate as shown by Fig 2.7. This model simulates the generation and transport of sputtered atoms and can be used as an input to SIMPROF or other simulators like SIMBAD. A flux distribution depends on sputtering energy, mass of the target material and the pressure of the sputtering chamber. SIMSPUD tracks the variation of all these factors and determines precise energy and angular distribution of flux species [44].

In the case of a cosine distribution the incident flux from the source is controlled by max_angle. This is represented by the width of the conically shaped angular distribution from the source point as shown by Fig 2.8 and can vary in width from 0 to 180°. The flux from particular incident point is restricted within the bounds of the cosine width and decreases as the emission angle diverges from the normal. The distribution is given by $\cos\left(\frac{\phi}{\phi_m} \cdot \frac{\pi}{2}\right)$ where ϕ is the emission angle and ϕ_m is the maximum angle of emission.

The cosine distribution approximates the angular distribution at the substrate. If we set a cosine width to 120°, as an example, than the range of an angular incident flux is from -60° to 60° with reference to the normal as shown by Fig 2.8.

Fig 2.7 Angular distribution of the sputtered atoms generated by SIMSPUD for Ti.

Fig 2.8 A cosine angular flux distribution from source point.

2.6 Visibility issues

One of the most important parts of the simulation process is to determine whether the flux from the source point landed on the receiving segment is shadowed. To determine if a source segment is visible to a target segment, we examine the flux from a point on the source to the target segment of the topography and determine if there is any segment in between blocking accessibility of the flux to the receiving segment. There are two types of visibility issues; two dimensional (2_D) and three dimensional (3_D), and we will explain each of them in detail.

2.6.1 Two dimensional visibility

In two dimensional simulations we use a line source to represent the source of the flux from the top of the simulation. The algorithm to identify the intersection of a line from the source segment to the target segment with a different segment when shadowing is occurring is divided into four parts;

- 1) a vertical flux line from the source to vertical segment on the surface of the substrate
- 2) a vertical flux line from the source to any segment on the substrate except vertical segment
- 3) Any non vertical flux line from the source to vertical segment and

- 4) Any slanted flux line from the source to any slanted segment as shown by Fig 2.9. This covers all the possible ways to express any flux line from the source to segment of any orientation on the substrate.

After setting up this type of algorithm, each line from a source segment to a substrate segment undergoes a series of tests to explicitly determine if any segment on the surface profile shadows the flux. Any line from the source which intersects with a surface segment other than targeted segment will not contribute any flux to the target segment. Since the source line is divided into m parts (see Section 2.3) through its length, the flux from each portion will be tested.

The total number of calculations regarding visibility will be computed as the following. For 2D case let us call x the number of segments on the surface and m be source segments, then number of computations (n) to test 2D visibility for all source segments will be $N = m \times x$ which is of the order of n^2 .

Fig 2.9 a) Vertical flux to vertical segment b) Vertical flux to any segment except vertical segment c) Any flux except vertical one to vertical segment and d) All slanted fluxes to slanted segments.

2.6.2 Quasi_three dimensional visibility

To locate exactly if any shadowing effect exists between an area on the plane source to the three dimensional symmetrical cylindrical surface which receives the incident flux, we need to set up an algorithm to determine the intersection of a line from the source area and a 3D surface other than intended target. As the surface is cylindrically

symmetrical a segment on the substrate to test for shadowing is rotated to generate a conic section. The entire 3D substrate surface can be divided into conic sections as shown by half cut surface view of Fig 2.10. Each segment in the profile is either horizontal, vertical or slanting surface which corresponds to discs, hollow cylinders or hollow cones respectively as shown by Fig 2.11 to Fig 2.13.

Using this description of the surface we can locate the centre of the substrate surface which is also the centre of the created conics whether it is a disc, cylinder or cone. Every segment on the surface other than the one all the flux from the source targets is tested for shadowing and each segment is considered as the objective target one at a time. If flux line hits any surface of a disc, cylinder or a cone shadowing is present and the flux from the source is not counted. Special routines are written to calculate the intersection point of the flux line and any segment on the surface other than intended target segment.

For the 3D case we can calculate the total computations required to test visibility as following; Let n be number of segments on the surface of the substrate as set by the user. We use only half of that segments ($n/2$) from one end to the centre point of the profile because of the symmetric characteristic it has and exact duplicate of flux in the first half of the source is added to the second half of the surface profile. The total computations (T) to test visibility in three dimensional case are $T = n/2 \times l \times m$ in the order of $O(n^3)$ where l and m are as defined in Section 2.3.

Fig 2.10 General half cut surface view that receives incident film having either disc, cylindrical or conical shapes.

Fig 2.11 Graphical representation of shadowing and non-shadowing effects of discs (flat surfaces).

Fig 2.12 Graphical representation of shadowing and non-shadowing effects of cylindrical segments.

Fig 2.13 Graphical representation of shadowing and non-shadowing effects of conical segments.

2.7 Visibility testing procedures in SIMPROF

We addressed the general idea of visibility in the two former subsections. In this section we will deal with how individual shadowing tests are performed.

2.7.1 Two dimensional visibility testing criteria

For 2D the flux lines and shadowing surface are both represented by lines. If there is no intersection between these lines flux reaches its target and is shadowed otherwise as shown by Fig 2:14. Specific routines are used to physically determine if an intersection exists or not.

Fig 2.14 Depiction of 2D shadowing effect, dotted flux lines are shadowed.

Fig 2.14 gives the general idea of shadowing in case of two dimensional simulation. However, we need to elaborate the idea in order to understand how shadowing is precisely determined. The algorithm to test visibility issue is divided into four cases. The simplest case is when the flux line and the substrate segment are both vertical or both horizontal. In either of these there will be no shadowing effect unless the two lines are coincident. The remaining three cases are; 1) segment is vertical and the flux assumes any direction but not vertical 2) flux is vertical and the segment assumes any direction but not vertical and 4) when both flux and segment lines are slanted.

In case 2 there will be no shadowing effect when the target and the source are both above h_1 or both are below h_2 as Fig 2.15a shows. Similarly when the abscissa of the source and the target are both smaller or both larger than the abscissa of the segment there will be no shadowing effect as shown by same figure. In all other instances of case 2 the intersection (x_c, y_c) of the two lines is calculated and the visibility is determined from there. To decide whether shadowing is there or not we test the position of the intersection. If the intersection point is above h_1 or below h_2 there will be no shadowing which will be otherwise as shown by Fig 2.15b. Case 3 is exactly the same as case 2 except the positions of the flux and segment lines are switched. Since a visibility test for case 3 behaves like that of case 2 we will not repeat it here.

During visibility test for both 2D and 3D surfaces we will use the following illustrations to represent source and target of the flux lines and intersection of the flux line with the substrate surface other than target (if it exists).

1. The source point will be represented by $\bullet$ T where T stands for target.
2. The target point will be represented by $\bullet$ S where S stands for source.
3. The intersection point will be represented by $\odot$

Fig 2.15 Visibility testing criteria of vertical segment and flux line a) Shadowing is not possible and b) Shadowing is possible.

In case 4 when both the source and the target are outside the box surrounding the segment as shown by Fig 2.16a there will be no possibility of shadowing. When the flux

lines cross the boundary of the box the intersection of the flux line and the segment is calculated. If the intersection (x_c, y_c) occurs outside the box there will be no shadowing as Fig 2.16b illustrates. However, if the intersection is within the box or its boundary specific tests have to be carried out to determine shadowing. That is if both the source and the target are above or below the intersection point there will be no shadowing as Fig 2.16b shows. Similarly if the abscissa of the target and the source are both less or both greater than the abscissa of the intersection point there will be no shadowing which will occur otherwise as Fig 2.16b shows. A special event in case 4 is when both lines are parallel. If the two lines are coincident shadowing occurs and not other wise.

Fig 2.16 Visibility testing criteria of slanted segment and slanted flux line for 2D
a) Shadowing is not possible and b) Shadowing is possible.

2.7.2 Three dimensional visibility testing criteria

In case of 3D as we outlined before we will divide the shadowing surfaces into three: Disc (ring), cylinder and a cone. The shadowing properties of each of these surfaces will be discussed separately. During a visibility test when both source and target points are above or below the shadowing surface there will be no shadowing effect as shown by Fig 2.17. All other cases will be tested individually.

Fig 2.17 Illustration of non shadowing effect for 3D when both source and target are above or below of the shadowing surfaces.

For the disc which is the simplest of all the remaining cases there is a possibility of having single intersecting point with each of the flux lines and the disc surface as shown by Fig 2.18. If the intersecting point is located outside the ring surface or inside the ring where it is greater than r_2 or less than r_1 there is no shadowing as illustrated by Fig 2.18a

otherwise shadowing effect exists as shown by Fig 2.18b.

Fig 2.18 Flux shadowing properties of a Disc where a) Flux is not shadowed and b) Flux is shadowed.

For cylindrical case the flux lines can cross one or two points on the horizontal surfaces of a height h_1 and h_2 or between them. When the radii of two intersecting points

are both greater or both less than the radius (r_1) of the cylinder there will be no shadowing effect. Similarly for single intersection point where the intersecting radius is greater than r_1 or is less than r_1 clearly there will be no shadowing as shown by Fig 2.19.

Fig 2.19 Non shadowing properties of cylindrical surfaces.

The shadowing effects of cylindrical surface are only possible when there is two

intersecting points of the flux lines with the cylindrical surface. When the radius of one of the intersecting points are greater than the radius (r_1) of the cylinder and the other is less than r_1 or vice versa clear shadowing will result as Fig 2.20 shows. There is one special case for cylindrical shadowing and will be dealt with later in this section due to its complexity.

Fig 2.20 Shadowing properties of cylindrical surfaces.

For conical case the flux lines can cross one or two points on the horizontal surfaces of h_1 and h_2 or in somewhere in between them. For two intersecting points when both the points are greater r_1 or both are less than r_2 of the cone there will be no shadowing as illustrated by Fig 2.21. For single intersection, if the radius of the intersecting point is greater than r_1 or less than r_2 or vice versa as shown by Fig 2.21 there will be no shadowing effect as well.

Fig 2.21 Illustration of conical non shadowing surface properties.

In case of shadowing there is possibility of having only two intersecting points of flux lines with the conical surface. If one of the intersecting points is smaller than r_1 and the other is greater than r_2 or vice versa shadowing will clearly be exhibited as illustrated by Fig 2.22. There is a special case remaining in the case of conical visibility test. This case is not simple and will be dealt soon.

Fig 2.22 Illustration of conical shadowing surface properties.

The visibility tests we conducted so far covered more than 90% of the required visibility tests. The remaining fraction of visibility tests needs more calculations for both cylindrical and conical surfaces to complete the tests. As shown by Fig 2.23 and Fig 2.24 flux lines traverse through cylindrical and conical surfaces. We need to know if these lines pierce through the surfaces or just pass over without touching any surface. To determine whether the traversing lines are shadowed or not we have to calculate the nearest point of these lines to the shadowing surfaces as the following,

$$m = \frac{z_1 - z_2}{x_1 - x_2} \quad m_n = \frac{-1}{m}$$

$$z = m \cdot x + b, \quad z_n = \frac{-x}{m}$$

Where m is the slope of the flux line, m_n is the slope of a line from the centre of the shadowing surface which is normal to flux line from the source to target, z and z_n are the equations of the respective lines as shown by Fig 2.18a. By equating z to z_n we can calculate

$$x_{min} = \frac{-b}{m + \frac{1}{m}}, \quad z_{min} = \frac{-x_{min}}{m},$$

$$y_{min} = \frac{y_2 - y_1}{x_2 - x_1} \cdot (x_{min} - x_1)$$

$$r_{min} = \sqrt{z_{min}^2 + (x_{min} - x_0)^2}$$

x_{min} , y_{min} and z_{min} are on the nearest point of the flux line to the centre of the shadowing surface and r_{min} is the length of the radius of the line from the centre of the shadowing surface to the nearest point of the flux line as shown by Fig 2.25a. Once r_{min} is known it is compared to the radius of the cylinder (r_1) of Fig 1.23 and if r_{min} is greater than r_1 there will be no shadowing.

Finally the special case concerning a conical surface needs more tests to be done before we can decide whether the flux lines shown in Fig 2.24 are shadowed or not. Since the surface radius of cone between h_1 and h_2 of Fig 2.24 is variable it is necessary to calculate such surface radius with respect to y_{min} of the flux line calculated before or y_{tar} we will determine this variable surface radius (r_{sur}) as following

$$r_{sur1} = r_2 + \frac{y_{min} - h_1}{h_1 - h_2} \cdot (r_1 - r_2)$$

$$r_{sur2} = r_2 + \frac{y_{tar} - h_2}{h_1 - h_2} \cdot (r_1 - r_2)$$

By using theorems of similar triangles we can calculate the variable surface radius on any point on the cone of Fig 1.25b. We have two different radii for same surface which may look confusing at the beginning. The reason is we have two different categories of

flux lines which create different surface radius. If the flux source is above h_1 and flux target is below h_2 of the shadowing surface or vice versa we use r_{sur1} otherwise we use r_{sur2} . Once surface radius of the cone is available two different tests are launched. When the source is above h_1 and target is below h_2 or other way round r_{min} is compared to r_{sur1} and if r_{min} is greater than r_{sur1} there will be no shadowing which will occur otherwise. On the other hand if the first intersecting point is less than r_1 and the target radius (r_{tar}) is less than r_{sur2} or vice versa there will be no shadowing effect otherwise the flux is blocked from its target.

Fig 2.23 Implicit visibility property of cylindrical surfaces.

Fig 2.24 Implicit visibility property of conical surfaces.

Fig 2.25 a) Determination of y_{min} and b) Determination of r_{sur} . The line marked with 1 and similar lines use r_{sur1} others use r_{sur2} .

2.8 Flux calculations with unity sticking coefficient (2D and 3D)

If we have unity sticking we only need to account for the flux from source segments. To add up the amount of flux striking a segment we must integrate the flux from all visible source segments. The angular distribution at the source, visibility and flux

transport are all needed to determine the flux arriving at a surface segment. The visibility and source description are as described above. To accumulate the flux transport the line from the source to target segment is partitioned into elements as shown by Fig 2.26. Each element (dx) of these partitions acts as an independent source. The flux line from that element makes an angle θ to the normal of the source segment. A line making an angle θ to the source segment and perpendicular to the flux line is as shown by Fig 2.26. The source element dx is projected to element dx_1 on that line. Another perpendicular line to the flux line is used on the target segment. The projected source element to that line is dx_2 . The perpendicular line to the target segment makes an angle α to the flux line from the source. The flux from the differential source elements to target will be calculated as following.

$$F = F(\theta) \cdot d\theta \cdot dx \quad \text{where} \quad dx = \frac{dx_1}{\cos(\theta)}$$

$$F_1 = F(\theta) \cdot d\theta \cdot \frac{dx_1}{\cos(\theta)} \quad \text{where} \quad d\theta = \frac{dx_1}{r} \quad \text{and} \quad dx_1 = d\alpha \cdot r$$

$$F_2 = F(\theta) \cdot \frac{dx_1 \cdot d\alpha \cdot r}{r \cdot \cos(\theta)}$$

$$dx_2 = dx_1 \text{ and } dx_2 = dx_3 \cdot \cos(\alpha)$$

$$F_3 = F(\theta) \cdot \frac{\cos(\alpha)}{\cos(\theta)} \cdot d\alpha \cdot dx_3$$

F_3 is the magnitude of the flux arriving the target from the source element. The amount of this flux is physically dependent on quantity of material from the source element, θ , α and r as illustrated by Fig 2.26. However, F_3 does not contain r because it had been eliminated through the derivation process. The quantity of the incoming flux from visible source segment is then explicitly given by

$$F_{ij} = dx_3 \cdot \int_{\phi_1}^{\phi_2} F(\theta_i) \cdot \frac{1}{\cos(\theta_i)} \cdot \cos(\alpha_j) \cdot d\alpha_j$$

Where θ_i is the angle at which particle is launched to arrive the intended segment with respect to the normal from the source segment and α_j is the angle between substrate segment normal and the incident flux as shown by Fig 2.26, $F(\theta_i)$ is the angular flux distribution of the source and F_{ij} is the magnitude of the flux reaching the j^{th} substrate segment from the i^{th} source segment. ϕ_1 and ϕ_2 are the initial and the final angles of the source segment to the target segment normal. The r dependence is contained in the integration. The total flux on certain segment from all the sources is

$$F_{inc} = \sum_{i=0}^{i=n} F_{ij} \cdot v_{ij}$$

Where v_{ij} is the visibility related number which is 0 if flux is not visible to the

target segment and is 1 if it is visible to it and n is the number of segments or areas from which flux is expected. θ_i and α_j of each point is computed by using dot product of vectors to fix their values. Calculating visibility (v_{ij}) in 2D for a single segment is $O(n)$ while it is $O(n^2)$ for a 3D segment. Flux calculations are more complex in 3D than in 2D as it involves more source points.

Fig 2.26 Depiction of how the flux transport from source segment to substrate segment is calculated.

2.9 Flux reflection models

When modelling the growth of thin films, produced by an incident flux, flux from the source is calculated taking into account any shadowing effect through the course of its travel. If the particle simply sticks on the substrate topography then the flux calculation is

done. However material that arrives the surface can reflect or re-emit depending on the type of the flux material, its energy and the condition of the surface.

If we wish to study the effect of sticking coefficient and re-emission we need to incorporate a model for reflection/re-emission [45]. Reflection refers to single or multiple bounces of depositing fluxes due to sticking coefficient less than unity. The sticking coefficient is the probability that the adatom is chemisorbed on the surface. Re-emission includes both reflection and desorption effects. Whenever there is a re-emission, a fraction of the precursors bounce back from the surface creating new angular distributions depending on the nature of the incident material and the surface.

Physically a number of reflection/re-emission models are possible. In general the flux re-emitted from the surface is a function of the incident angle and energy. There are two extreme cases for the interaction between the growing surface and the incident material. In one case the re-emitted material is not a function of the incident angle and re-emits with a cosine distribution. In the second case the surface acts like a mirror, a perfect reflecting surface, and the particle re-emits at an angle equal to the incident angle from normal of the surface. We model a number of different kinds of reflection/re-emission phenomena that we refer to as **no_reflection**, **diffusive-lossy**, **chemical**, **specular_lossy**, **specular and resputtering** as shown by Fig 2.27. Material from the original source, reflected or re-emitted flux from the substrate itself are all considered as source material. To simplify the modelling of growth with remission we limit the program to 6 specific reflection/remission models [46].

1) No reflection: That refers to unity sticking and all incoming flux is adsorbed on the surface immediately.

2) Diffusive -lossy: The source flux strikes the surface adsorbing a part of it and reflecting the remainder. The re-emitted flux is at very low energy and does not cause any more re-emission. The angular distribution of the re-emitted flux is cosine. Physically this process is like a loose trapping on the surface of high energy incident flux and is a single bounce process.

3) Chemical-Diffusive: All flux has a probability of sticking (S_c) and is re-emitted with a cosine distribution. This model is a multiple bounce process and physically is modelling chemical deposition on a surface.

4) Specular-Lossy: Source flux is assumed to be at a high energy and upon striking the surface has a probability of sticking. If it does not stick it reflects specularly. At reflection the flux is assumed to lose energy and the remitted flux has a unity sticking coefficient. This process models low pressure sputter deposition of refractory metals and is a single bounce model.

5): Specular: This model assumes all the attributes of specular lossy model except high energy fluxs are reflected. It is as a multiple bounce model.

6) Resputtering: Resputtering is a high energy flux bombardment of the surface of the growing film which causes resputtering of the previously deposited material. This can

be achieved by supplying high energetic ions to the growing surface. Re-emission probability is determined by ion energy, angle of incidence and relative ion to atom mass. The distribution of the resputtered flux can be specular or cosine depending on ion energy, film material and surface profile. This is generally a single bounce model.

Fig 2.27 Thin film deposition models a) All incident flux sticks to the surface (Unity sticking), b) Diffusive-lossy model, c) Diffusive-chemical model, d) specular_lossy model, e) Specular model and f) Resputtering model.

2.10 Flux calculations with reflection in 2D using iteration

With reflections the quantity of flux received by each segment is dependent on the total amount of reflected flux from all other segments and from the original source. In

general if reflections are present then we can consider two sources of flux material for each node, one from the incident points and other from all other nodes and we have

$$F_I^i = F_{inc}^i + \sum_{j=0, j \neq i}^m (F_I^j)(1 - S_c) = F_{inc}^i + F_r^i$$

Where F_{inc} is the total incident flux from the source received by node i. F_I^j is the total flux received by j^{th} nodes, F_r^i is the total reflected flux obtained by node under consideration (node i) from all other nodes (j nodes) and F_I^i is the total flux obtained by node i on a single bounce. This equation represents a set of m coupled non linear equations that need to be solved to determine the flux F_I^i at each node. We solve this set of equations using iteration, the subscript n denotes the iteration number

$$(F_I^i)_n = F_{inc}^i + \sum_{j=0, j \neq i}^m ((F_I^j)_{n-1})(1 - S_c)$$

Where i and j denote the flux receiving and the reflecting nodes respectively, n and n-1 keep track of current and previous iterations required to solve the number of equations set by the iterative process. Adding all the components of the flux received by each node we have formulated a set of equations to conduct all the necessary calculations to estimate the amount of flux reflecting from each node of the surface topography.

With a single bounce algorithm iteration is not needed because of the termination of the reflection at first bounce. However, in a multiple bounce an algorithm to terminate the

iteration through the process of calculation is required. The equations are solved iteratively as an approximate measure to obtain all the required information within reasonable tolerance. The deposited flux at each node is then calculated as:

$$F_d = F_l^i \cdot S_c$$

Where F_d is the flux expected to deposit over intended segment. Whenever reflection occurs from substrate surface the total computations regarding visibility issue increases from $N = m \times x$ as stated in Section 2.6.1 to

$$N = m \times x + \sum_{i=0}^{i=n} x \cdot (x-1)$$

For each iteration, where n is the number of times that reflection is iterated and this is time consuming.

2.11 Flux data structure

For the unity sticking and diffusive reflection it is only required to keep track of the magnitude of the flux striking a segment. This is due to the fact that the reflected flux distribution is only a function of the magnitude of the incident flux. However, for the specular and resputtering models we need to know the flux distribution on the segment to determine the reflected flux. Because of this it is needed to store the incident flux distribution for each segment.

To store the flux of each node efficiently we created an appropriate array in the data structure to store the flux distribution at each segment. All fluxes from different source points to same segment are added to this distribution. The distribution is stored as an array of 36 bins covering 180^0 .

2.12 Surface diffusion

The adatom flux striking each segment can now be calculated but could still move due to diffusion. Diffusion is a process in which particles move from regions of high concentration to regions of low concentrations as a result of their thermal motion. There are three types of diffusion which are volume, grain boundary and surface diffusion. Volume diffusion occurs in the interior of the material while grain boundary diffusion relates to movement at the interface of polycrystalline crystals and surface diffusion takes place on the surface of the material. When a material is depositing on the surface at a high temperature, vacancy and the surface diffusion can both take place. However, if the surface is at a low temperature surface diffusion dominates. We believe that surface diffusion dominates in the kind of work we are doing, and volume and grain boundary diffusion is ignored.

The dependence of the diffusion constant upon temperature can be written as function of temperature (T) and the activation energy for the surface diffusion (E_{ad}).
[46,47]

$$D = D_0 \cdot e^{(-E_{ad})/(kT)}$$

Where D is the diffusion constant, D_0 is the frequency factor or pre-exponential factor and relates to the lattice vibrations and k is Boltzmanns constant. Diffusion length can also be expressed as $L = (2 \cdot D \cdot t)^{1/2}$, where t is average length of time for which the diffusing material was on the move. The equation governing the surface diffusion can be written as

$$\frac{\delta c}{\delta t} = D \cdot \nabla^2 c + \frac{c}{\tau} + F$$

Where the term $(\delta c / \delta t)$ represents the concentration change with time, c is the physisorbed adatom concentration, $\nabla^2 c$ is the concentration divergence, c/τ is the term arising from material adsorption in to the surface and F is the source material to the growing surface from the incident flux.

To solve this equation we use a finite difference method applying an explicit central difference approximation (Fig 2.28), and the differential equation becomes

$$\frac{(c_i^n - c_i^{n-1})}{\Delta t} = \frac{D(c_{i-1}^n - 2 \times c_i^n + c_{i+1}^n)}{\Delta x^2} - \frac{c_i^{n-1}}{\tau} + F$$

Where c_{i-1}^n and c_{i+1}^n are the amount of material on previous and the next nodes respectively, c_i^n is the current concentration of material on the node under consideration and c_i^{n-1} is the previous concentration on same node and D is the diffusion constant. Rearranging the terms and making c_i^n the subject of the formula we have.

$$c_i^n \left(1 + \frac{2 \cdot D \cdot \Delta t}{\Delta x^2} \right) = \left(1 - \frac{\Delta t}{\tau} \right) \cdot c_i^{n-1} + D \cdot \frac{\Delta t}{\Delta x^2} \cdot (c_{i-1}^n + c_{i+1}^n) + F \cdot S_c \cdot \Delta t$$

then the equation becomes

$$c_i^n = \frac{B}{A} \cdot c_i^{n-1} + \frac{C}{A} (c_{i-1}^n + c_{i+1}^n) + F \cdot \frac{S_c}{A} \cdot \nabla t$$

$$\left(A = 1 + 2 \cdot D \cdot \frac{\Delta t}{\Delta x^2} \right) \quad \left(B = 1 - \frac{\Delta t}{\tau} \right) \quad \left(C = D \cdot \frac{\Delta t}{\Delta x^2} \right)$$

Fig 2.28 Central difference approximation.

Solving the last equation systematically we can determine specific quantity of physisorbed matter on each segment on the surface and chemisorbed amount. The rate of surface diffusion increases exponentially with τ and with decreasing activation energy. At higher temperatures, higher surface diffusion is expected and this will affect the film structure.

Having determined the amount of flux chemisorbed by each node on the topography surface we can develop an algorithm to add the calculated mass to the film. After adding that mass on the surface the first layer of film is created. As the surface advances the calculating procedure starts from the beginning to compute the next layer's mass and looping continues until the intended thickness is reached.

2.13 Surface evolution

The goal of all the analysis in this chapter, is to determine the amount of flux striking the surface of the topography profile, the diffusion rate and the amount of matter being added to each segment. This matter must now be added to the surface. To accomplish proper surface evolution, certain criteria have to be followed to obtain a physically sound film growth. A robust correct growth algorithm has to be chosen to move the segments. A number of options are available in choosing a growth direction in which surface nodes move. These algorithms calculate the growth directions using parameters such as segment normal, node normal and average mass to be added for each segment. The actual surface advancement mechanisms must move the nodes in a way to ensure conservation of the added volume and material mass. As the surface grows or contracts new nodes are added or removed, so as to maintain reasonable density on the surface. Surface advancing techniques will be discussed in detail in the next chapter.

Chapter 3

3.1 Surface movement algorithms

An understanding of the evolution of surface features under deposition or etching processes is of considerable practical importance to integrated circuit fabrication. To date, a number of surface evolution methods have been proposed for microelectronic manufacturing. Some of these methods will be briefly discussed next.

1) Huygens principle: Huygens' original principle states that every point of a wave front may be assumed as the source of secondary wavelets which spread in all directions with speed equal to the speed of propagation of the waves. This principle can be applied to track the motion of any physical front whose normal speed to the surface is known at all points. This can be constructed by assuming an envelope of waves constructed by a set of discs of some radius, r , centered on the initial surface at a specific time [49]. Circles centered on the original surface boundary that have moving fronts with velocity vector, v , as their radii as shown in Fig 3.1. All the circles are then connected together to delineate surface growth at a particular time [50]. This technique reproduces the expected growth profile with respect to its original surface from which it was grown.

Fig 3.1 Illustration of the entropy condition of Huygens' principle.

2) Shock-tracking method: This method uses nodal points connected by linear segments to model the evolving surface. The surface of the topography is represented by a function which explicitly defines its position and boundaries at a given time. However, unlike a number of geometric models existing, the movement of nodes and segments are controlled by a change in slope between two adjacent pair of nodes. In this method, propagation of each nodal point is tracked to identify if the surface curvature has discontinuity or not. The velocity vector of each point of the surface is determined by its normal component [51]. At some instants, where the surface function ceases to be differentiable an entropy condition identifies the solution and singularity problems are resolved [52]. Discontinuity points are called shocks.

3) Level-set: Level set methods are another way used to advance surfaces and the

formulation is based on solving a Hamilton-Jacobi type equation for a propagating level set function velocity of surface normal [53,54,56]. This method offers an accurate way for tracking interfaces under complex motions to handle topological merging and breaking naturally. The central idea is to view the moving front as a particular level set contour of higher dimensional function. Numerical methods allow level set method to accurately predict the effect of advancing surface issues. Where shocks on the surface occur, the necessary entropy condition is invoked to give reasonable solution. Three types of fronts; downward, upward and flat fronts are commonly used in this method. In level set, the problems from these fronts are satisfactorily solved by using entropy conditions.

4) Rule-based methods: In this method a discrete parametrized version of the interface boundary is used [53,56,57]. In 2D the surface is a set of nodes and segments and in 3D a set of facets are used. The positions of nodes and segments are updated by moving the surface by a set of rules based on the matter to be added. This type of model is quite accurate, but has problems with handling the propagation of surface corners (convex and concave corners) correctly. Removing such problems is considered in our string based program, SIMPROF, which falls in this category. Concave corners are handled by using a geometrical approach to stabilize surface motion and to avoid discontinuity problems. The other problem which emerges in rule based schemes, convex corners, uses maximum velocity variations through the periphery of the corner to overcome the problem. Both cases are equivalent to Huygens principle and work effectively. A significant problem with rule based methods is the determination of the angle of growth of each node. If this is not

chosen correctly surface irregularities will form.

3.2 Film growth modeling

Inorder to simulate the growth of thin films, a simulator must model three basic phenomena [53] which are determining the magnitude of the flux striking each segment, diffusion of this flux along the surface profile and incorporation of the adatom flux into the surface. The film is then advanced according to the surface structure and the appropriate mass is added to each segment. A fundamental physical phenomenon that must be modeled to obtain a correct thin film is to determine the direction and magnitude of growth of the surface at each specific instant. This must be known to determine the growth direction of each node on the surface and to move each point on the surface along a vector to the location of the new surface. It is very difficult to obtain all the detailed information needed for a growing film due to the complexity of the film structure and some kind of approximations are generally adopted.

There are several simple growth situations that we use to insure a simulated film that adequately predicts real films. The parameter which has the largest effect on thin film morphology is the adatom mobility [36]. We will summarize real film growth under low and high adatom mobilities.

3.3 Low mobility

If the incident flux sticks where it hits and does not diffuse significantly on the

surface the surface growth is dominated by the incident flux distribution and shadowing [58]. When a film is deposited at low temperature with respect to its melting temperature, a microstructure consisting of individual columns separated by voids and grain boundaries is generated [59]. For real films it has been observed that the film density decreases with increasing angle of incidence as shadowing increases and voids between columns widens [36]. The effect of oblique angle deposition on substrate at low temperatures increases film porosity caused by the shadowing effect. Deposition sources for microelectronics processing are oriented in such a way that the flux arrives perpendicular to the wafer, but for small topographical features such as via sidewalls, the flux may arrive highly obliquely. This effect may lead to a localized low density and could create regions susceptible to failure.

During the growth of a columnar microstructure in a vapor deposited thin films the surface advances along the surface normal at velocity related to the orientation of the surface. For obliquely incident fluxes of low mobility the columnar structure of the film grows in an off normal direction as illustrated by Fig 3.2. A question arises, is the surface moving vertically or at the angle of the columns? A simulated film from SIMBAD with limited mobility is shown in Fig 3.3.

Fig 3.2 Columnar structure of a film grown from obliquely incident flux

Fig 3.3 Simulated film from SIMBAD.

Although the surface moves obliquely the film grows normal to the original surface. For string based models, modeling oblique incident flux complicates the growth by possibly moving surface nodes obliquely as shown by Fig 3.4. During growth some nodes will then leave the edge of the simulation region.

Fig 3.4 Nodes move in the direction of the incident flux

3.4 High mobility

The fundamental concept behind high temperature processing is to increase the self diffusion rate of physisorbed atoms during deposition or post deposition annealing [43,48,57]]. This can either be through mechanisms of surface or bulk diffusions. In the case of significant surface diffusion deposited matter will be moved tangentially on the surface.

Increasing the substrate temperature during deposition and consequently increasing the diffusion length leads to a film consisting of larger columnar grains with smoother surfaces [58,59] as illustrated in Fig 3.5. The incoming precursors experience a long interaction with the surface and lose memory of the incoming particle trajectories. The surface growth will be normal to the surface and the surface velocity is proportional to the local adatom concentration.

Fig 3.5 A smoother columnar film structure grown from obliquely incident flux at high diffusion.

3.5 Deposition over topography

The deposition of a flux over topography such as a trench provides a number of simple tests for growth algorithms. A vertical deposition (over trenches) using either directed sputtering or evaporation and a low surface diffusion should produce the growth shown by Fig 3.6a. Such profiles have good bottom coverage and zero step coverage. Problems will possibly arise from the growth direction of the profile corners. As shown by Fig 3.6a and b growth on corners should not produce any sidewall growth. Significantly improved sloped step coverage is as shown in Fig 3.6c. Such improvement is the result of the sloped profile. Although bottom coverage has kept its nominal value, step coverage has significantly improved due to the slope of the trench sidewalls. For zero diffusion the step coverage is proportional to $\cos(\theta)$ as shown by Fig 3.6c.

Fig 3.6 Dependence of deposition on topography structure and direction of flux. a) Vertical wall trench b) Depiction of corner growth of a and c) Sloped wall trench.

3.6 Uniform deposition

If a very high diffusion length or very low sticking coefficient is present then the deposition rate will be uniform over the entire topography. A situation that could occur in high temperature deposition [58,59] or some CVD deposition [60,61,62]. This situation is also a good test of a growth algorithm. Since the actual flux depositing on to a surface is dependent on several factors like visibility, surface structure, sticking coefficient and complex flux integrations, we will force a uniform flux deposition to test uniform film growth. This sets the amount of volume to be deposited on each point on the surface as a

constant and is used to test surface growth at corners as Fig 3.7 shows.

Fig 3.7 Uniform deposition through surface topography.

3.7 SIMPROF's growth modeling

The surface of the growing film has to be advanced in the proper direction to simulate correctly the deposition of the incoming flux species and to match real films deposited for integrated circuit fabrication processes. At low mobilities growth orientation depends on the incoming flux direction as seen in the previous sections. A robust general growth angle algorithm is needed. Once surface velocity and growth direction are determined for each point on the surface it is moved accordingly.

Segment size is a very important parameter in string based models. If the segment size is very small simulation time will be very long, but the surface growth will advance correctly because the surface velocities change little from segment to segment. By using larger segments simulation time will decrease with respect to segment length. However that will complicate the rules used to advance the surface as the surface velocity directions

differ greatly from segment to segment. With large segments concave and convex surfaces must be handled carefully to get correct simulations. If the segment length is much less than diffusion length as in the case of high mobility, the growth direction may be assumed to be normal to the surface.

As we defined before, a surface in SIMPROF is a geometrical specification represented by a set rectangular coordinates. A method of calculating the amount of material arriving at particular segment was considered in earlier chapter to determine the quantity of flux on each segment and the volume Δv to be added in the time Δt . This quantity is then added to the serially chained segments across surface of the topography and the first layer of the film is formed from the initial surface. The direction of growth of each node is controlled by the growth angle.

During the simulation the surface evolves with time and as fresh material arrives on the newly created surface layers, we update the contents of the variables in the nodal data structure for the additional growing film layers and determine the quantity of material to be added to the segment of the new layer. Layers are then created on top of each other to simulate the whole film growth. This process continues until the thickness of the growing film attains that requested by the user. As the surface develops, the newly created surface may need to have more nodes on some areas and less on others to keep nodal density reasonable. As the surface grows segments are removed or added as needed to maintain the desired resolution.

During growth the film is not immune from irregularities being formed by surface looping which will distort the growth from its normal course producing an incorrect result. To eliminate this problem, specific routines are created to remove loops and restore the normal surface growth. These routines search for the intersection of the loops and quickly eliminate the unnecessary loops but keep the surface intact. The importance of this emerges if you carry out simulation with loops allowed and one using overlap removal as shown by Fig 3.8.

Fig 3.8 Simulated films from SIMPROF a) With overlaps and b) With overlaps being cleaned up.

Several different methods are adopted in this program to investigate the best possible way that we can associate the growth direction and velocity to the incident flux and surface structure. Each of these methods has its own unique way to define a particular

growth orientation to decide the relative direction for which the surface is to grow. A number of ways are used to test the general behavior of growing surface with respect to theoretical expectation. Three simple algorithms to determine the growth angle were investigated using the node normal, the average flux direction and the two adjacent segment normals weighted by the volume to be added to each segment. As shown below all of these growth models fail the basic tests. Finally a modified weighted segment normal model which produces acceptable results will be discussed.

3.7.1 Surface evolution toward node normal

The simplest growth orientation is to use node normal growth. Let point(x,y) be on the surface that receives flux. Consider points(x1,y1) and (x2,y2) on the surface which are previous and next nodes with respect to reference node at point(x,y) respectively as shown by Fig 3.9. The node normal (θ_n) is then given by

$$\theta_n = \text{atan} \frac{(y2 - y1)}{(x2 - x1)} + \frac{\pi}{2}$$

where θ_n gives surface growth direction. Similarly we can calculate segment normal (θ_{s1}, θ_{s2}) by considering the segments located on either side of reference node which are actually previous and next segments. Segment normals are then computed as following

$$\theta_{s1} = \text{atan} \frac{(y - y1)}{(x - x1)} + \frac{\pi}{2} \quad \text{and} \quad \theta_{s2} = \text{atan} \frac{(y2 - y)}{(x2 - x)} + \frac{\pi}{2}$$

where θ_{s1} and θ_{s2} are previous and next segment normals respectively as verified

by Fig 3.10 and will be used in the next section.

Fig 3.9 Depiction of how node normal is calculated.

Fig 3.10 a) How segment normal is determined by using isolated segment and b) Depiction of growth direction with respect to growth angle.

For surface growth governed by a node normals the surface topography normals are

calculated for each segment and each node. These angles are used to direct the movement of whole growth of the surface as long as the film is growing. The procedure of normal growth depends only on the characteristics of surface topography prior to the deposition of new film on the surface. The rate of change of surface depends on surface velocity $v_s = \frac{\Delta m_i + \Delta m_{i-1}}{\Delta l_i + \Delta l_{i-1}}$ where Δm_i and Δm_{i-1} are the amount of mass deposited on the previous and next segments with respect to reference node and Δl_i and Δl_{i-1} are the corresponding lengths. A growth G vector for each node is $\hat{G} = v_s \cdot \Delta t \angle \theta_G$ where v_s is the velocity and θ_G is the growth direction as shown by Fig 3.11b. During deposition as the surface evolves, the surface shape changes and new layers are formed, creating new topography which controls the new direction of growth. This trend continues until the required film is attained.

Although this model of growth angle satisfactorily simulates uniform and high diffusion models as illustrated by Fig 3.11a and 11b it fails to correctly simulate low diffusion vertical flux growth as shown by Fig 3.11c because it does not even closely approximate to the expected output shown in Fig 3.11d. The reason is the convex corners of the profile does not grow properly. This is due to using a node normal for θ_G which uses only surface geometry to determine growth angle as shown by Fig 3.11e. This algorithm requires the surface to grow in a direction of $\left(\frac{\theta_{s1} + \theta_{s2}}{2} \right)$ with respect to reference node. During that growth, the growth direction ignores the interaction of the segment surface velocity and surface topography to determine the correct direction of growth.

Fig 3.11 Simulation output using node normal growth direction at distribution angle of 1° and unity sticking a) Uniform growth b) High diffusion growth c) Zero diffusion growth d) The expected output for zero diffusion growth and e) Depiction of why part c of the Fig 3.11 failed

3.7.2 Film growth with respect to average flux direction

When the node normal was used to control thin film growth movement, only the surface structure was used to guide node growth and it failed because it does not account the flux direction for low mobility growth. Now we will use a different approach which uses the average flux direction incident on each of the surface profile. That flux can be obtained from both the incident flux from the target and any reflected flux from the surface profile itself. We calculate the average flux direction at each segment as

$$\phi_{ave} = \left(\sum_{j=1}^{36} \frac{\left(j + \frac{1}{2}\right) \cdot f_j}{F_t} - 18 \right) \cdot 5 \cdot \frac{\pi}{180}$$

Where f_j is the amount of flux in a specific bin of the flux distribution data structure and F_t is the total flux for a particular segment.

Fig 3.12 Relation between flux distribution over bins and average flux direction.

The growth vector for each node on the surface will be $\hat{G} = v_s \cdot \Delta t \angle \theta_G$ where v_s is the velocity vector, Δt is the time of growth and $\theta_G = \phi_{ave}$ for this case.

Fig 3.13 shows two different views of thin films simulated from SIMPROF by using average flux growth direction. Although this model works for low diffusion with vertical flux as shown by Fig 3.13a, it completely fails for high diffusion as shown by Fig 3.13b. The use of an average flux direction and ignoring the surface topography is obviously incorrect for cases of high diffusion. It creates numerical instability and distorted growth.

Fig 3.13 Simulation outputs from SIMPROF using average flux direction at distribution width of 1° a) Zero diffusion simulation output and b) Highly diffusive.

3.7.3 Thin film growth with respect to segment mass weighted average direction

The primary concern of the film growth algorithm is to ensure the nature in which the incident flux is generally deposited produces good growth characteristics. In order to achieve that goal two basic things must be taken into account. First, the geometry of the surface must be considered to influence the direction of the expected growth and secondly the amount of flux deposited on nearby segments should be considered. These two factors are then used to determine the growth angle and surface velocity. In the next model the two adjacent segment normals and the mass (Δm) on each segment are used to determine the direction of surface growth vector using a mass weighted average of the two segment

normals. This type of growth is more complicated than previous growth models and still presents difficulties for some cases.

This growth model can be divided into three cases which will be explained as following. In case one, if the flux on the segments to each side of the reference node is zero, the growth angle will be defined as the node normal and the surface will not be advanced at all as Δm is zero and therefore the surface velocity will be zero. Secondly, if the flux of one segment is zero the growth angle will be the nonzero segment normal and its velocity will be $\frac{\Delta m_i}{\Delta l_i}$. Thirdly, if the flux on both segments is not zero, some calculations must be done to define the growth angle direction. For the last case, let mt_1 and mt_2 be the added masses per unit length on the two segments at both sides of the reference node and total mass $mt = mt_1 + mt_2$. The weighted average growth directions of x and y of the growth vector can then be computed as following.

$$x = \frac{mt_1}{mt} \cdot \cos(\theta_{s1}) + \frac{mt_2}{mt} \cdot \cos(\theta_{s2}) \text{ and } y = \frac{mt_1}{mt} \cdot \sin(\theta_{s1}) + \frac{mt_2}{mt} \cdot \sin(\theta_{s2})$$

Where θ_{s1} and θ_{s2} are previous and next segment normals and n , n_1 and n_2 are reference, previous and next nodes as shown by Fig 3.14.

Fig 3.14 This figure depicts how weighted mass average is calculated a) When mt_2 is zero b) When mt_1 and mt_2 are not zero for concave surface and c) When $mt_1 = mt_2$ for convex surface.

The growth angle θ_G will be $\theta_G = \text{atan}(y,x)$ with surface velocity of $v_s = \sqrt{x^2 + y^2} \cdot \Delta t$. This kind of computation is carried out on each node on the surface profile and growth angle is set on each time to regulate thin film growth on that node. On very concave corners it is found that the growth angle is occasionally at nearly right angles to the correct growth. This occurs when one segment has little or no flux striking it. To find

a solution for the problem we find the direction in which each segment is growing and determine if the growth angle we calculated lies in between the two segments. If not we recalculate the growth angle forcing it to stay its proper place in between the two segments. This regulates film growth and allows it to advance in a direction relative to relative weights of x and y to fix the new growth angle. Fig 3.16 shows simulation output from SIMPROF using this growth model and distribution width of 1° . This model simulates uniform growth and high diffusion correctly as shown by Fig 3.16a and b but it fails to correctly simulate zero diffusion with vertical deposition as illustrated in Fig 3.16c. Failure at concave corners necessitates a search for a new growth model as this type of model is not robust due to complicated non physical rules in handling the concave corners.

Fig 3.15 Depiction of deviated and corrected growth angles.

Fig 3.16 Simulation output using weighted mass growth direction at distribution angle of 1° and unity sticking a) Uniform growth b) High diffusion growth c) Zero diffusion growth and d) The expected output of c.

3.8 Failure of the attempted growth modeling

The main goal of developing growth model is to achieve a method that consistently allows SIMPROF to simulate the advancing surface correctly in a reliable manner. We attempted three different models to fulfill that idea and a number of simulations were conducted using each of the models, to evaluate their validity. Simulation outputs were

then analyzed carefully and each of the models failed in one way or another. To correctly predict the evolution of the surface profile and its response to the flux variation over the topography, we attacked the growth model from a different perspective. This new venture will be explained in the following section and is a modified weighted mass average algorithm.

3.9 Basic algorithms for advancing surface

The main goal of these models is to get an accurate, stable and efficient technique to advance the surface for different physical structures and depositing fluxes to guarantee correct surface evolution. Every surface structure can be subdivided into three different regions. These regions can be classified as flat, convex and concave surfaces.

3.9.1 Flat surface

Let us focus our attention on a flat portion of the surface as it is the simplest of the three cases. Let mt_1 and mt_2 be the amount of mass received by segments s_1 and s_2 respectively and n , n_1 and n_2 be the reference, previous and next nodes as shown by Fig 3.17. The growth angle for this type of surface is calculated as the node normal growth angle and the surface growth vector of the advancing flat surface is equivalent to $\hat{G} = v_s \cdot \Delta t \angle \theta_n$. where $v_s = \frac{mt_1 + mt_2}{l_1 + l_2}$ and l_1 and l_2 are the respective lengths of previous and next segments. This type of growth satisfies Huygens' principle.

Fig 3.17 Model of modified weighted mass average growth angle for flat surface.

3.9.2 Convex surface

On convex surface the segment velocity v_{s1} is proportional to mt_1 and v_{s2} is proportional to mt_2 , but segment 1 and segment 2 have to be connected carefully as the surface advances because of the behavior of the convex surface. As shown by Fig 3.18a the convex corner has to be advanced in a way that conserves matter. If the surface is advanced using a straight line connecting A to C as shown by the light solid lines of the same figure, mass is not conserved. In order to conserve mass, the material deposition has to be reduced from mt_1 and mt_2 on either side of the reference node in a smooth manner creating a rarefaction fan. As mt_2 decreases while mt_1 is kept constant the growth angle approaches toward 90° where there will be a vertical growth as Fig 3.18 indicates.

The convex corner grows as the dashed line of Fig 3.18 illustrates. The surface velocity of the growing surface changes from velocity $v_{s1}(mt_1)$ to velocity $v_{s2}(mt_2)$ of the

previous and next segments with respect to reference node. The growing surface of the convex corner can be advanced in two ways. In the first case, to obtain smooth transition from v_{s1} to v_{s2} during growth a linear transition from is used. Where an arbitrarily chosen parameter (τ) to control the growth movement has to be determined. This parameter is calculated as $\tau = \frac{\theta_G - \theta_1}{\theta_2 - \theta_1}$ where θ_1 and θ_2 are the normal angles to previous and next segments of the convex corner with respect to reference node. θ_G is the growth direction of the convex node and remains as was modeled by weighted average mass of section 3.7.3. The amount of flux on the advancing surface is proportional to the rate of change of corner volume and can be formulated as $d = v_{s1} \cdot (1 - \tau) + v_{s2} \cdot \tau$ where d is the distance that the surface advances in the direction of growth angle. The actual growth vector of the growing surface is $\hat{G} = d \cdot \Delta t \angle \theta_G$. The second possibility is to use the maximum velocity vector to determine the growth of convex corner and $d = \max(v_{s1}, v_{s2})$, while the growth angle remains as above. In either case a rarefaction fan results which connects the left states to right states while conserving matter through its surface. Both ways produce similar results, but SIMPROF uses the second case for its simplicity.

Fig 3.18 Expected growth from modified weighted mass average growth angle for convex surface a) When $mt_1 = mt_2$ b) When $mt_2 < mt_1$ and c) When $mt_2 \ll mt_1$.

3.9.3 Concave surface

The last case of the three is concave corner which could be as shown in Fig 3.19. To advance this type of surface in such corner is not a trivial matter and is where the weighted average method failed. It needs careful formulation to advance to the next correct surface. Conceptually the next and subsequent surface of the growing film should have same

structure (corners) as the original surface as shown by Fig 3.19 In contrast to convex corner, this corner produces a smaller volume than expected volume and to conserve the incoming flux, the volume has to be increased to accommodate all additional material and to conserve matter. Point d is geometrically determined as following

$$y_1 = mt_1, \quad b = \frac{mt_2}{\sin\left(a - \frac{\pi}{2}\right)} \quad \text{and} \quad (y_2 = m_2 \cdot x + b)$$

at intersection of line y1 and line y2,

$$x = \frac{y_1 - b}{m_2} \quad \text{and} \quad d = \sqrt{x^2 + y_2^2}$$

as shown by Fig 3.20, then the growth angle (θ_G) can be calculated as $\theta_G = \theta_1 - \beta$ Where θ_1 is normal angle of the previous segment and angle $\beta = \text{atan}(y_2, x)$. Generally, someone may say surface advancement of this corner is only determined geometrically, but actually this may be calculated as

$$d = \sqrt{\left(mt_1 - \frac{mt_2}{\sin\left(a - \frac{\pi}{2}\right)} \right)^2 + mt_2^2}$$

which is just another way of saying the geometrical interpretation is just equivalent to flux proportions on either side of reference node. Surface growth vector of each node is

then calculated as

Again this model is equivalent to Huygens principle

as shown by Fig 3.20.

In this concave case, d which is the distance that the surface advances from the reference node in the direction of θ_G is fixed and then growth angle is calculated and used to determine the direction of growth.

In the previous other two cases (flat and convex surfaces) the growth angle remains same as that modeled by weighted mass average while a new growth angle is calculated for a concave surface. After using this type of growth angle modeling, SIMPROF's simulation outputs agrees with theoretical expectations of the program as shown in Fig 3.21. If sticking coefficient (S_c) is less than unity, step coverage improves due to reflecting fluxes as shown by parts a2, b2 and c2 of Fig 3.21. Likewise, if diffusion is allowed to take place the model works quite nicely as shown by parts a3, b3 and c3 of Fig 3.21. At the same time this type of growth angle models uniform deposition very well as shown by Fig 3.21e. This kind of growth model exhibits robustness, reliability and the program uses it as its reference growth model. In Fig 3.21 Dep width stands for deposition width and S_c stands for sticking coefficient.

Fig 3.19 Expected growth from concavely formed corner of a growing film.

Fig 3.20 Flux geometry depicting how the surface is advanced in concave corners.

Fig 3.21 Simulation outputs from SIMPROF with a1) $Sc=1$, Dep Width $=1^\circ$ at zero diffusion a2) $Sc=0.5$, Dep Width $=1^\circ$ at zero diffusion a3) $Sc=1$, Dep Width $=1^\circ$ with diffusion b1) $Sc=1$, Dep Width $=90^\circ$ at zero diffusion b2) $Sc=0.5$, Dep Width $=90^\circ$ at zero diffusion b3) $Sc=1$, Dep Width $=90^\circ$ with diffusion c1) $Sc=1$, Dep Width $=180^\circ$ at zero diffusion c2) $Sc=0.5$, Dep Width $=180^\circ$ at zero diffusion c3) $Sc=1$, Dep Width $=180^\circ$ with diffusion and e) uniform deposition.

3.10 Film density

For thin film growth over topography variation of film density is inevitable. The density of the deposited thin film varies with average incident angle of incoming flux due to shadowing effect of the topography. The density drops substantially as the deposition angle becomes more oblique [39,63,64]. To incorporate this in SIMPROF a model of density is needed as a function of average incident angle and width of the flux distribution on each segment on the surface topography. These two parameters (ϕ_{ave} , ϕ_w) are used to characterize the density function. The density model can be determined experimentally or from a microstructure model such as SIMBAD. Then for each segment on the surface the volume $\frac{\Delta m}{\rho}$ added to the surface is calculated where ρ is the density of the added material. As the surface grows the corners on the top of the surface shadow more flux on some points on the surface and create more density variations as shown by Fig 3.22. The faster growing neighboring regions create a continuous formations of regions with low densities.

The density of the film deposited over the side walls of via or trench is lower than the density of the film on top horizontal surfaces and on the bottom [38,39]. The side wall film has considerable lower densities dropping toward the bottom as opposed to higher density horizontal film as shown by Fig 3.22. There will be a significant increase in step coverage if tapered side walls are used and the density of the film deposited on the side walls is clearly improved due to less oblique flux created by the structure of the via or trench as shown by Fig 3.22.

Fig 3.22 Simulated films from SIMPROF using distribution width of 60° with $Sc = 0.5$
a) thin film depiction on stepped topography b) Exhibition of density variation of (a), c)
Thin film depiction on slanted topography and d) Demonstration of density variation of
(c).

3.11 Reliability of the model

The main task of SIMPROF is to demonstrate reliable simulation of thin film deposition. Most of that job is complete at this time but it needs some way to verify the

validity of this work. One important step to implement such verification is to show the compatibility of SIMPROF to other existing models. In the next chapter we will demonstrate how well simulation outputs from SIMPROF agree with those of already existing models and real films from processing labs.

Chapter 4

4.1 Validation strategy

The first step toward the validation of SIMPROF will be to perform a few simple tests to compare to SIMBAD and a simple level set program to SIMPROF. These tests will provide a preliminary judgement of how SIMPROF behaves compared to these other two simulators.

To further test the validity of SIMPROF we intend to carry out large number of simulations using both SIMBAD and SIMPROF and compare their results. SIMBAD has been verified in number of technical and scientific papers and has a practical application in industry. SIMBAD is therefore a suitable tool for us to use as a reference model to measure the validity of SIMPROF. Initial topographies for both SIMBAD and SIMPROF are described by identical test.init files. Each simulator performs its simulation until a set thickness of film to be deposited is reached. Simulated film outputs from both simulators will be closely analysed and compared to see if they match. If they differ the reason for the difference will be determined. Two categories of simulations will be conducted to study how closely the output of this simulator match to that of SIMBAD. Two dimensional simulations will be discussed first, considering a variety of cosine distributions and sticking coefficients. Three dimensional simulations will be compared following the same procedure. Finally experimental films will be compared to SIMPROF simulation outputs to provide a true test of the model. A brief description SIMBAD and

level set programs will follow. SIMPROF has of course been described in detail through this thesis.

4.2 SIMBAD

The basic SIMBAD program is a two dimensional Monte Carlo simulator developed to model the growth and microstructure of thin films deposited over topography [43]. The basic model accounts for the effects of the vapour flux shadowing and surface diffusion by the adatoms. These are the most important factors in determining the step coverage and the columnar microstructure for refractory films. In SIMBAD, the film is represented by an aggregation of 10^4 and 10^5 identical hard discs [58]. Each of these discs represents the statistically averaged behaviour of large number of film atoms (typically 1000 per disc). These discs are serially launched from just above the growing film and follow straight line trajectories until they strike the substrate or the film. The discs aggregate into the film after short surface diffusion to minimise the surface curvature-dependent chemical potential. The combination of ballistic shadowing and short range surface diffusion successfully accounts for the formation of the columnar thin film microstructure characteristic of refractory metals. Without extensions, the basic 2D SIMBAD model is suitable for simulating deposition in a long feature such as a trench. The simplest 3D extension of SIMBAD exploits cylindrical symmetry (quasi-3D) and represents the film with a single 2D slice through the topography [43,64]. Density and stoichiometric profiles of the films can be obtained by averaging a large number of simulation slices.

4.3 Level set

Level set methods are numerical techniques for computing the position of the propagating fronts. They are specifically designed for profiles which can develop sharp corners, change of topology and undergo order of magnitude change in speed. The central idea of this method is the formulation of a correct equation of motion for a front propagating with curvature dependent speed. These equations are based on solving a Hamilton-Jacobi type equation to obtain the actual velocity of the evolving curvature [66]. As the propagating surface evolves it can develop corners and discontinuities which require a weak solution in order to proceed correctly. A weak solution is a mathematical term used when solving discontinuity. The correct weak solution comes from enforcing an entropy condition similar to the one in gas dynamics or to the hyperbolic conservation law for the propagating interface. By using the appropriate type of numerical solution and entropy condition, where applicable, any type of surface can be evolved smoothly whether the thin film is deposited or etched from the surface.

A simple 2D Level set program was written, in which a surface velocity is defined and the surface is evolved. No flux calculations are done and it is only suitable for simple tests such as uniform growth and vertical deposition.

4.4 Verification procedure

Fig 4.1a and d show how the SIMPROF, SIMBAD and Level set respond to vertically deposited flux with no diffusion. Likewise, Fig 4.2 illustrates a uniformly

deposited film from each of these simulators. SIMPROF responds to a vertically deposited flux with no diffusion over the vertical topography as shown by Fig 4.1a. There is no lateral growth on the side walls because with zero diffusion the vertical sidewalls of the topography do not receive any flux and as a consequence only flat/horizontal surfaces of the topography are advanced. The corners of Fig 4.1a grew as expected. Level set simulation produces slightly rounded corners with no diffusion as Fig 4.1d indicates. This slightly deviates from the expected growth of the corners but is acceptable otherwise. This is due to the definition of the surface normal at the corner. It is not possible to use SIMBAD with no diffusion and it displays lateral growth due to this.

With equal amount of diffusion both SIMPROF and SIMBAD produce similar outputs as indicated in Fig 4.1b and c respectively. The only significant difference between the films is the sharp corners present in SIMPROF simulation. The SIMBAD algorithm implicitly causes a local minimization of surface curvature which is not present in SIMPROF and produces a smoothing of the film.

Similar topographies of Fig 4.1 are again used to test how each of the three simulators responds to uniform deposition. As Fig 4.2 indicates all the simulators respond reasonably to uniform deposition. The convex corners of SIMPROF, SIMBAD and level set are equivalently rarefied as shown by Fig 4.2a, b and c respectively. The concave corners, flat and vertical surfaces of all the simulators approximately grew according to the original topography structures. SIMPROF, SIMBAD and level set have produced uniformly deposited films that are sufficiently matched.

Fig 4.1 Vertically deposited films a) Simulation from SIMPROF with no diffusion, b) and c) Simulations from SIMPROF and SIMBAD at low diffusion, and c) Simulation using level set program.

Fig 4.2 Uniformly deposited films a) Simulation using SIMPROF b) Simulation using SIMBAD and c) Simulation using the level set program.

4.5 SIMPROF's validation

The primary concern of the following section is to show how well the simulation outputs from SIMBAD and SIMPROF match to the extent we can ensure whether SIMPROF is behaving correctly. The focus is to determine the percentage of step and bottom coverage produced by each simulator. The bottom and step coverages of each simulator are then compared to each other for an initial verification of SIMPROF's reliability.

A series of simulations were conducted in each simulator to collect the necessary information for such a comparison. During these simulations, deposition widths varying from 1° to 180° in steps of 45° and sticking coefficients from 0.2 to 1 in steps of 0.2 are used to obtain large amount of data for both simulators. The information obtained from these simulations were then plotted to easily compare results from simulation outputs.

The actual simulations will be divided into three categories: Two dimensional (2D) simulations with varying deposition widths and constant sticking coefficients and 2D simulations of varying sticking coefficients and constant deposition widths; three dimensional (3D) type of varying deposition widths and unity sticking coefficient; and a third case regarding the comparison of experimental films to SIMPROF and SIMBAD simulations.

A few examples of simulated films will be shown prior to plotting coverages. These figures help to get an idea of how the simulated films from both simulators are matched.

Fig 4.3 to Fig 4.6 show how the bottom and step coverages and overall appearance of the simulated films change with the distribution width and sticking coefficient of each simulation. The sharp top corners of simulated outputs from both simulators are slightly different. That is due to a surface curvature minimization used by SIMBAD. SIMBAD can also display anisotropic film growth at top corners as it has tendency to grow the film preferentially at 60° to the surface volume due to the use of hexagonal packing.

Fig 4.3a and b show simulations using unity sticking coefficient and a narrow distribution width of 1° . Both figures have thick bottom coverage and zero step coverage. Keeping the sticking coefficient unity and increasing the distribution width to 45° shows improved step coverage and slightly decreased bottom coverage as shown by Fig 4.3c and d. By varying the sticking coefficients and distribution width a set of simulated films were produced from both simulators as shown by Fig 4.3 to Fig 4.6. By specifically looking at Fig 4.4a and b we can see a nearly conformal coverage through the surface of the trenches. This is due to lower sticking coefficient and if we decrease it further still better coverage may be obtained. Generally, to get a uniform film over the surface of trenches or vias a low sticking coefficient or high diffusion is necessary. A large number of such simulations were performed and the data extracted from them is presented in the following section.

Fig 4.3 Illustration of how SIMPROF and SIMBAD simulation outputs in 2D are comparable to each other a) and b) Are SIMPROF and SIMBAD simulations respectively at a distribution width of 1° and unity sticking coefficient and c) and d) Are simulation outputs from both simulators respectively at a distribution width of 45° and unity sticking coefficient.

Fig 4.4 Illustration of how SIMPROF and SIMBAD simulation outputs in 2D are comparable to each other a) and b) Are SIMPROF and SIMBAD simulations respectively at a distribution width of 90° and unity sticking coefficient and c) and d) Are simulation outputs from both simulators respectively at a distribution width of 90° and 0.4 sticking coefficient.

Fig 4.5 Illustration of how SIMPROF and SIMBAD simulation outputs in 2D are comparable to each other a) and b) Are SIMPROF and SIMBAD simulations respectively at a distribution width of 135° and 0.2 sticking coefficient and c) and d) Are simulation outputs from both simulators respectively at a distribution width of 180° and 0.4 sticking coefficient.

Fig 4.6 Illustration of how SIMPROF and SIMBAD simulation outputs in 3D are comparable to each other a) and b) Are SIMPROF and SIMBAD simulations respectively at a distribution width of 1° and unity sticking coefficient and c) and d) Are simulation outputs from both simulators respectively at a distribution width of 180° and unity sticking coefficient.

4.5.1 Validation of SIMPROF in 2D through variation of deposition width and constant sticking coefficients

In Fig 4.7 and Fig 4.8, two plots show the step and bottom coverage as the deposition width is varied while sticking coefficient is kept constant for 1.0 and 0.5. Sidewall (step) coverage for both simulators increases from minimum (approximately 0) to maximum as the deposition width increases from 1° to 90° and then decrease linearly by falling from maximum to some value (but not to zero) as the deposition width moves from 90° toward 180° . Both coverages are very much dependent on the distribution width and sticking coefficient. As the deposition width increases from 1° , the side wall is exposed to more flux and step coverage starts to improve. But this trend does not continue indefinitely and step coverage starts to drop at deposition width greater than 90° . The main reason for that is the sharp shrinking of the profile opening as the film grows for deposition width greater than 90° which reduce the amount of flux reaching the steps. Step coverages of both simulators match reasonably well as shown by Fig 4.7.

Fig 4.7 Depiction of step and bottom coverage versus deposition widths at unity sticking coefficient.

The bottom coverage of both simulators start at higher percentage (around 100%) of the nominal thickness on flat surfaces at very small deposition width and continuously drop as the deposition width increases until it becomes 22% of the nominal value at 180° . For smaller deposition width, bottom coverage is almost equal to that of a flat surface because the incident material is released in a direction almost perpendicular to the bottom surface. At deposition width of 1° SIMPROF's coverage is about 7% higher than that of SIMBAD as shown by Fig 4.7. From Fig 4.7, it is clear that bottom coverages of both simulators are satisfactorily equivalent showing a comprehensive match.

Fig 4.8 Depiction of bottom and step coverages versus deposition widths at sticking coefficient of 0.5.

Fig 4.8 is identical to Fig 4.7 except it has sticking coefficient of 0.5 rather than 1 allowing some of the incident flux (50%) to reflect from the surface. Similar observations identical to those done on Fig 4.7 are carried out on Fig 4.8 reveal both step and bottom coverages of the two simulators are proportional and well matched as shown by Fig 4.8. From Fig 4.8, it is clear that bottom and step coverages are larger than those of Fig 4.7, particularly bottom coverage is larger than nominal flat surface thickness (more than 100%) and the reason is due to reflection. By comparing Fig 4.7 to Fig 4.8, one can immediately recognize the effect of reflection on bottom and step coverages. As shown by Fig 4.8, both simulators exhibit improved step and bottom coverages which is a

primary concern of submicron processes. This makes the issue of reflection an important step to demonstrate flux deposition of different materials having different characteristics and will be pursued more in the next section.

4.5.2 Validation of SIMPROF in 2D through variation of sticking coefficients and constant deposition width

So far we varied deposition width while maintaining sticking coefficient at a constant value one at a time. Now by keeping deposition width at some unique value for each set of simulation and varying the sticking coefficients from 0.2 to 1 at steps of 0.2, several plots are given by 2D simulations.

The first of these figures, Fig 4.9, at deposition width of 1° and varying sticking coefficients shows step and bottom coverages of SIMBAD and SIMPROF. As the sticking coefficient decreases, both coverages increase as expected due to the incident flux reflected from the surface. At smaller sticking coefficients and at smaller deposition width bottom coverages are greater than 100%, see Fig 4.9, and that is because it receives all incident flux from the source as well as reflected flux from all topography surfaces exposed to the bottom. Thus sticking coefficients less than unity can strongly influence conformal coverage. As we move from smaller deposition width to larger ones, step coverage increases while bottom coverages decreases as shown from Fig 4.9 (dep width of 1°) to Fig 4.11 (dep width of 90°). Beyond 90° both bottom and step coverages begin to drop at such larger deposition width as shown by Fig 4.12 and Fig 4.13. Bottom

coverage is higher than 100% at deposition width up to 45° as shown by Fig 4.9 and Fig 4.10 and less than 100% beyond 45° as Fig 4.11 to Fig 4.13 indicate. This coverage sharply falls at larger deposition width as shown by Fig 4.11 to Fig 4.13, but in any case both coverages drop from higher to smaller values. All the figures from Fig 4.9 to Fig 4.13 of both simulators (SIMBAD and SIMPROF) exhibit very well matched simulation outputs and that once more verifies the validity of SIMPROF simulator.

Fig 4.9 Depiction of bottom and step coverages versus sticking coefficients at deposition width of 1° .

Fig 4.10 Depiction of bottom and step coverages versus sticking coefficients at deposition width of 45° .

Fig 4.11 Depiction of bottom and step coverages versus sticking coefficients at deposition width of 90° .

Fig 4.12 Depiction of bottom and step coverages versus sticking coefficients at deposition width of 135° .

Fig 4.13 Depiction of bottom and step coverages versus sticking coefficients at deposition width of 180° .

4.5.3 Validation of SIMPROF In 3D under unity sticking coefficient and varying deposition width

Fig 4.10 is created from 3D simulations having the same specifications as Fig 4.7. After careful inspections, both simulators show very comparable step and bottom coverages. Both coverages of Fig 4.14 are considerably smaller than those of Fig 4.7 except at sharp deposition width. The reason behind that is the shadowing effect of 3D is much more dominant than in 2D and less flux is allowed to reach the side and bottom walls. All these figures confirm the validity of SIMPROF through varying distribution widths and sticking coefficients.

Fig 4.14 Depiction of bottom and step coverages versus deposition widths at unity sticking coefficient.

4.6 Verification of SIMPROF with respect to experimental films

We will now deal with a comparison of SIMPROF and experimental films to create an acceptable proof for the validity of SIMPROF.

An evaporated film of Tungsten deposited over a high aspect ratio trench is shown in Fig 4.15. Although evaporation produces a highly directional flux that is perpendicular to the substrate surface, the evaporated flux energy is very low and for tungsten (which has a high melting point) diffusion will be small [67]. Fig 4.15b and c present SIMPROF simulations with and without the density algorithm while Fig 4.15d is from SIMBAD. Both simulated films were produced by using narrow 1° cosine distribution width with a unity sticking coefficient. By comparing the simulated films to experimental film in Fig 4.15a, it is clear that the simulation outputs from both simulators are well matched to the experimental film. Fig 4.15b is different from the experimental film because it does not account for the density as the experimental film does. As the deposition angle becomes more oblique the density drops substantially. The average density of simulated films using grey scale has lighter regions representing a lower density [38]. The lower density regions of thin films have thickness greater than corresponding higher density regions because the mass of the lower density regions is distributed to a larger volume.

Another set of experimental and simulated films are shown in Fig 4.16. A radio frequency (RF) sputtering system with large target and at significant operating pressure was used as the source of the film. The uniform erosion and large target of this system

produces a flux with broad angular distribution [67]. A SIMSPUD angular distribution and unity sticking coefficient were used to produce the simulated films. As shown by Fig 4.16 simulated films from SIMPROF and SIMBAD compare well to the experimental film. Simulation of the density effect is less important for broad flux distribution than oblique flux distributions as shown by Fig 4.15 and Fig 4.16 respectively.

In Fig 4.17 films deposited over high aspect ratio trenches from a small target sputter system at a pressure of 8 mTorr are shown. Due to the non uniform erosion of this target and the small target diameter the angular distribution is much narrower [67,68]. Thus, the adatom flux of this system is highly directional as the experimental film displays. Both simulators show no mushrooming effect and the lack of mushrooming in SIMBAD is not an algorithmic problem as originally anticipated. The problem appears to arise from a physical effect as was proposed in [67]. For that reason the expected notches on the top of the simulated film is absent from both simulators, Fig 4.17c-d, and are considerably different from the experimental film of Fig 4.17a. Otherwise the simulated films are clearly matched to the experimental film. Another film deposited by a same system but at a pressure of 14 mTorr is presented in Fig 4.18. The mushrooming effect is appearing from this Fig 4.18a as well, but the additional gas scattering has broadened the angular distribution and the notch is less noticeable. Simulated films from SIMPROF and SIMBAD, shown by Fig 4.18b-d, are reasonably matched to the experimental film of Fig 4.18a due to less severe notching produced by the more pressure.

Fig 4.15 Evaporated films a) SEM picture b) Simulation from SIMPROF with constant density c) Simulated film with non-uniform density from SIMPROF and d) Simulated film from SIMBAD

Fig 4.16 Sputtered films a) SEM picture b) Simulated film from SMPROF with constant density c) Simulated film with non-uniform density from SMPROF and d) Simulated film from SIMBAD.

Fig 4.17 Sputtered films a) SEM picture of 8 mTorr b) Simulation from SIMPROF with uniform density c) Simulated film with non-uniform density from SIMPROF and d) Simulated film from SIMBAD.

Fig 4.18 Sputtered films a) SEM picture of 14 mTorr b) Simulation from SIMPROF with uniform density c) Simulated film with non-uniform density from SIMPROF and d) Simulated film from SIMBAD.

4.7 Verification of SIMPROF using high aspect ratio topographies

With high aspect ratio vias and trenches the deposition of an effective thin film barrier layers becomes quite difficult. In this section we will test how SIMPROF simulation results are comparable to SIMBAD and to experimental films using such high aspect ratio features.

Fig 4.19 shows an experimental film, a SIMBAD simulation and three SIMPROF simulations results which illustrates the effect of low film density on the surface profile. The SIMBAD simulation is a single slice through the film and clearly shows the low density on the film of the side walls. The first SIMPROF simulation assumes a uniform film density of one and it is clearly seen that the sidewall thickness is much too small. Introducing a non uniform film density calculated from the local incident flux distribution increases the sidewall thickness by a factor of two (Fig 4.19d). This is, however, insufficient and a resputtering model must also be used to produce a good match to the SEM (Fig 4.19e). The SIMBAD simulation of Fig 4.19b assumes resputtering is present as does the corresponding SIMPROF simulation of Fig 4.19e and both simulation results are quite consistent with the SEM photograph of Fig 4.19a [17].

Fig 4.19 a) SEM film of TiW film b) Single SIMBAD simulation showing porous sidewalls. Line segment simulations. Unity sticking coefficient c) Homogenous film density of 1.0 d) Density determined from local sputter flux distribution and e) With resputtering model present.

4.8 Verification of SIMPROF by using experimental films on overhang structures

Overhang structures are suitable test models to investigate non-unity simulation using SIMPROF. Ti, W and TiW films were deposited over these structures and each of these depositions will be discussed and experimental and simulated films will be compared.

The sputtered Ti displays no deposited film under the overhang as shown by Fig 4.19a and is well modelled by the simulated films from SIMPROF and SIMBAD as shown by Fig 4.20b-d. For the titanium simulations an angular distribution from SIMSPUD is used and no Ti film was visible beneath the overhang indicating a unity sticking coefficient. As can be seen from the figures the simulations correspond very accurately to the experimental result. The evolving surface profile predicted by SIMPROF and SIMBAD closely follow that of experimental film as shown by Fig 4.20.

Sputtered Tungsten deposited on an overhang structure shows a small degree of re-emission beneath the overhang. The W was assumed to reflect specularly due to its heavy mass. The simulated films were produced by using an effective sticking coefficient of 0.7 and user defined distribution width. The simulated profiles from SIMPROF and SIMBAD show a good match to the experimental result as shown by Fig 4.21.

The experimental TiW sputtered film displays the most significant film on the bottom of the over hang as illustrated by Fig 4.22a. In order to successfully model this

film the W was assumed not only to undergo specular reflection at 0.7 sticking coefficient but also causes resputtering of Ti which is weakly held to the growing film surface. Simulations from SIMPROF and SIMBAD were carried out under sticking coefficient of 0.4 using TiW and user defined distribution widths. Both simulation outputs closely match to the experimental film as shown by Fig 4.22a-c. The film visible beneath the overhang is clear evidence of the occurrence of re-emission or resputtering. This concludes the comparison of simulated films on overhang structures with respect to experimentally produced films on same structures. The comparison of experimental films to simulated films from SIMPROF have shown SIMPROF's power as a valid simulator.

We have performed large number of simulations from SIMPROF and SIMBAD during validation procedure of SIMPROF and a considerable number of experimental films were also prepared. All simulations from SIMBAD and all experimental films were than compared to SIMPROF simulations and the output results were carefully analysed. SIMPROF's simulations reasonably matched to simulations from SIMBAD and to experimental films as well. This is a clear indication to SIMPROF's validity as a simulator.

Fig 4.20 Experimental and simulated thin films of Titanium on overhang structures a) experimental film b) and c) Simulated films with and without density from SIMPROF and d) Simulated film from SIMBAD. Unity sticking coefficient was used during simulations

Fig 4.21 Experimental and simulated thin films of Tungsten on overhang structures a) Experimental film b) and c) Simulated films with and without density from SIMPROF and d) Simulated film from SIMBAD. Re-emission coefficient of 0.7 is used during these simulations.

Fig 4.22 Experimental and simulated thin films of Titanium and Tungsten on overhang structures a) experimental film b) and c) Simulated films with and without density from SIMPROF and d) Simulated film from SIMBAD. Re-emission coefficient of 0.4 is used during these simulations.

Chapter 5

5.1 Conclusion

A crucial step to manufacture VLSI and ULSI integrated circuits is the fabrication of reliable thin films during processing. The SIMPROF program developed in this thesis has successfully simulated thin film growth over variety of two dimensional and three dimensional topographies.

In chapter 1 the methods and uses of thin film deposition is thoroughly explained. A number of techniques that can be used for thin film simulation are discussed and the role of metallization in VLSI design and several types of deposition methods are briefly reviewed. Film growth and related properties are then concisely described. Contact creation and its significance to reliability of deposited thin films is also reviewed. This chapter generally describes the behaviour of thin film deposition and growth.

SIMPROF uses a string algorithm to model the growth of thin film in 2D and 3D surfaces. The main features of SIMPROF are explained in chapter 2 to give a view of how the topography surface is created and represented geometrically. 2D and quasi 3D algorithms are described and thoroughly tested to obtain correct simulation results. Although reflection and re-emission from the topography surface is considered in 2D, the 3D model does not consider for it. The data structures, models of the incident flux sources, visibility issues, flux distributions, flux data structures and surface diffusion are all dealt within this chapter. All flux calculations and related mathematical models have

been described in this chapter.

Once the amount of mass to be deposited on specific node on the substrate surface is computed the surface must be advanced in a way that insures proper surface growth in an appropriate direction. All growth related computations are described in chapter 3. Several surface movement techniques such as level set, Huygens' principle, shock-tracking and string based algorithms are briefly discussed at the beginning of the chapter. A number of growth modelling algorithms such as node normal, average growth direction and weighted mass average growth are tested and found to lack full reliability. A modified weighted mass average is then used to give the correct growth direction. This type of growth modelling divides the substrate surface into flat, convex and concave surfaces. Each of these three cases uses a unique algorithm to develop the appropriate growth direction and the surface is advanced accordingly. The effect of low and high surface mobility on the advancing surface topography is considered. Uniform and non-uniform depositions are used as test cases. Film density is another important issue that uses mass-volume relationship to adjust the surface movement. As the shape of the topography changes the film density can change creating some regions of low densities and affecting the growth profile. To incorporate a density function ρ into SIMPROF an average incident angle and flux distribution width on each segment of the surface topography is used. The ratio $\frac{\Delta m}{\rho}$ of each segment is then calculated to determine the specific growth volume on each segment throughout the topography surface.

As the surface is advanced the thin film takes shape on the topography surface. To make sure the reliability of SIMPROF as a simulator it is absolutely necessary to review and compare its results with that of other existing simulators and with experimental films. In chapter 4 we compare a number of simulation outputs from SIMPROF to SIMBAD and experimental films to establish the validity of SIMPROF.

The comparison of SIMPROF to SIMBAD and experimental films ranges from simple films with unity sticking coefficient to more complex films. Complex films encompass a number of issues such as reflection/re-emission, specular, diffusivity and resputtering modes. However, SIMPROF does not model mushrooming effect and that is physical effect rather than algorithmic problem. The lack of mushrooming was originally thought to be an algorithmic problem, but later found it was a physical problem. Experimental results on overhang structures compared to simulation results from SIMPROF are also closely matched and that shows the validity of SIMPROF. After comparing large number of simulation outputs from SIMPROF to SIMBAD and experimental films we obtained the required support for the validation of SIMPROF.

5.2 Recommendation for further work

This program has successfully modelled thin film deposition on 2D and 3D surfaces. There are three areas for further work to enhance SIMPROF. Although reflection/re-emission model was considered in this program for 2D it lacks a reflection/re-emission model in 3D and it is necessary to include such a model into SIMPROF in

the future. For simulating deposition into vias it is very important to consider reflection in 3D surfaces. The other areas which need incorporation of further work in SIMPROF is the inclusion of an etching model and models of energetic biased diffusion. Adding these three models to SIMPROF will allow to fully simulate deposition and etching of 2 and 3 dimensional topographies.

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