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**Simulation and modeling of the structure and
surface profile of sputtered refractory films for
VLSI barriers**

by

Mohammad Salahuddin

**A thesis submitted to the
Faculty of Graduate Studies and Research
in partial fulfilment of the requirements
for the degree of
Master of Engineering**

**Ottawa-Carleton Institute for Electrical Engineering,
Department of Electronics,
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January 5, 1998

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submitted by Mohammad Salahuddin

in partial fulfilment of the requirements for

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Abstract

This thesis will present a new model for sputtered thin film growth of refractory metals based upon the atomic momentum of sputtered particles arriving at the substrate. The new model is incorporated into the original SIMBAD application to simulate certain phenomena of thin film growth that were previously not addressed.

Experimental metal films were sputtered on trenches/vias to a thickness of $1\mu\text{m}$. Tungsten was the primary metal used for most of the experiments. Analysis of metal films showed that lateral growth at the corners of the trenches/vias constantly exceeded simulation results obtained using previous SIMBAD models. The modified model takes into account motion of sputtered atoms due to their momentum after reaching the growing thin film surface. The new SIMBAD algorithm successfully produces thin films that closely depict experimental results including lateral growth features. A number of films were simulated using different conditions with the modified SIMBAD model to show the universality of the lateral growth phenomenon.

Acknowledgement

I want to thank my parents, Mr. M. A. Sattar and Mrs. Monowara Begum, for their love and hard work which has been responsible for my success. My wife Annie, Shopon, Koke, Mohammad Hafiz, Shahida Hafiz and friends have been a constant source of support and I am grateful to them.

I wish to convey sincere and deep appreciation for my thesis supervisor Dr. Tom Smy for being cool and easy to work with. I also thank him for his patience, encouragement and excellent ideas. A special thanks goes out to Dr. N.G. Tarr for helping me whenever I needed it(which was often).

Without Lyall, Carol and Yaz I could not have produced the experimental results required for this thesis. Thanks guys. A note of appreciation must be conveyed to Dr. Steve Dew, Dr. Steve Winterton, Dr. R. N. Tait, Dr. M. Brett, Dr. Chan(SEM lab), Peter(SEM lab), Dr. Tan and Khalid Sheerger for their experimental assistance, creative ideas and suggestions.

I also want to thank the department of electronics at Carleton University and the Alberta Microelectronics Center for their financial support.

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Chapter 1

Introduction

1.1 Motivation

Development of both the transistor and electronic computer have shaped today's high-technology based modern society. Since the first polycrystalline germanium transistor was built in 1947[1], staggering advances in I.C. technology have resulted in exponential growth of the number of transistors that can be put on a single chip. Rapid improvements in the design and fabrication of solid state devices and integrated circuits have been fueled by the continued reduction of transistor dimensions, which have decreased from centimeters down to microns(Fig. 1.1).

Very Large Scale Integration (VLSI) requires the interconnection of more than 10^5 devices per chip. With the feature size of VLSI (Very Large Scale Integration)

Figure 1.1: Illustration of (a) increase in components per chip over time and (b) phenomenal decrease of minimum feature length.

circuits becoming ever smaller, concern about reliability has increased considerably. The metallization of an integrated circuit plays an important role in determining the reliability of the circuit. Metallization is the process method used to connect individual device elements to one another on a silicon chip with metal layers and can account for a large portion of the chip area; more than 60% in some devices[2]. Metallization results in conductive metal or metal-like layers over VLSI topography. In microelectronics, metal lines are used to supply power and transmit information carried by electrons. Beyond supplying power and communication links between different devices on a chip as well as devices and the outside world, metallization

must provide control to device characteristics, such as Schottky barrier height, contact resistance and MOS properties[3].

As feature sizes have decreased, voids, insufficient step coverage and other defects in metallization techniques and materials have negatively impacted the reliability of VLSI circuits. It has been estimated that up to 80% of failures in a VLSI circuit can be attributed to metallization defects[4]. Understanding the development of thin film growth for metallization has become paramount to the chip manufacturing process. The main objective of this thesis is to analyze and model the behaviour of thin film growth over VLSI topology for the sputtering process - currently the most popular method of VLSI metallization. Particular focus is placed on barrier layer deposition of refractory metals and 'unusual' growth features.

1.2 Metallization

Today the metal stack often consists of several metal layers(Fig. 1.2) each requiring a process deposition step. Multiple layers and materials are used to enhance device performance and lifetimes by mitigating fabrication problems that can occur. Ti is often used as an initial layer to improve adhesion to the Si or oxide surface. The next metal level is a protective barrier layer used to prevent 'spiking' or encapsulate the fill material.

The solid solubilities between a sputtered metal and substrate material can give

Figure 1.2: Multilevel metallization stack.

rise to 'spiking'. For example, due to the solubilities of Al and Si, interdiffusion reactions between them can often result in junction 'spiking' where Aluminum can penetrate deep into the Si device. This problem has been partially solved by using Al-Si alloys as opposed to just pure aluminum, but the problem of Si precipitation still exists in device contacts that do not utilize a barrier metallization layer[5].

Encapsulation is required when the interdiffusion of materials can result in one of the materials being 'poisoned'. Copper diffused into Si results in deep level traps in the band structure which can lead to junction leakage. Barrier integrity and notching are far more serious issues for Copper thin film deposition than for Aluminum thin film deposition. To completely isolate a copper fill layer from the Si or silicon oxide, the copper layer is encapsulated using a refractory metal such as W or Ta(Fig. 1.3).

A wide variety of materials such as W, TiW or TiN are used for barrier layers.

Figure 1.3: Depiction of Copper fill encapsulation.

Electrically the fill layer is the most important and is responsible for delivering the functional requirements(power delivery and communications) of metallization.

Fill layers should meet the following requirements:

1. Low electrical resistivity,
2. Easy to form and pattern,
3. Minimal electromigration.

The metal chosen for deposition will determine the fundamental material characteristics. No metal is optimal for every criteria outlined above, but aluminum (Al)

does meet most of them and is the material most often used for interconnect metallization. Aluminum has a low resistivity which allows circuits to operate at high frequencies due to low RC(Resistor-Capacitor) delays. However, Aluminum does present some problems from a fabrication standpoint. Aluminum has a very low melting point which can cause a number of concerns in fabrication and performance at higher temperatures.

Si/Al precipitates increase contact resistance and have a negative effect on electromigration performance of interconnects. To enhance electromigration performance of interconnects Cu is added to the Aluminum; typically about 0.5 percent to effectively reduce electromigration degradation. Amounts higher than 0.5 percent cause problems in dry etching, corrosion and reliability degradation. Hillock formation (stress relief mechanism) and voids are also negative issues associated with Al interconnects. Despite these problems, current metallization schemes are successful in making Al interconnects more robust by adding layers like Ti to improve adhesion to the Si device contacts and barriers layers like W, TiW or TiN.

Recent research developments suggest that Copper might be the metal of the future. Preliminary research indicates that Copper has superior electromigration resistance than Aluminum alloy metallization. Copper(Cu) has been suggested as a replacement for Al alloys due to its higher conductivity. These two facts combined might force Copper metallization to be used for high speed small feature applications.

The ability to drive capacitive loads with higher current densities may improve circuit speed[6].

1.3 Methods of Deposition

The deposition technique chosen can not change the fundamental material characteristics but can be optimized to obtain enhanced film characteristics from an application point of view. Several factors determine the deposition technique chosen:

1. Material to be deposited,
2. Blanket or selective deposition,
3. Equipment required and its availability
4. Deposition rate and throughput
5. Final purity level and film properties,
6. Sensitivity of the deposit to the deposition environment,
7. Step coverage desired and aspect ratios used,
8. Equipment cost,
9. Equipment maintenance cost,

10. Unit product cost.

There are two broad classifications for VLSI metallization deposition techniques: chemical vapour deposition(CVD) and physical vapour deposition(PVD).

1.3.1 Chemical Vapour Deposition(CVD)

Chemical vapour deposition can be defined as the process of stable compound formation on a heated substrate by the thermal reaction or chemical decomposition of gaseous compounds. The reaction, whether it is a compound that will decompose because of thermal energy to give the desired film or a set of compounds chemically reacting to form the film, must take place only at the wafer surface. Partial or total reactions in the gas stream above the wafer can create “fluff” and other forms of particulates which can result in films with low density and many pinholes. For IC manufacturing the most useful CVD reactions are almost always characterized as surface catalyzed. This implies even though reactants may be present in the gas ambient above the wafers and at the same temperature as the wafers, the reaction should occur on the hot wafer surface and on any other hot surfaces, but not in the gas stream.

CVD techniques can be utilized for deposition of amorphous, polycrystalline, or single-crystal (epitaxial) layers[7]. The process is commonly used to deposit semiconductor passivation, diffusion barrier and conductor layers[8]. For I.C. manufacturing,

CVD dielectric deposition is extremely important[9]. There are several types of CVD deposition techniques of which low pressure CVD (LPCVD) is the most popular. Plasma etched CVD (PECVD), is used to create ions that recombine to give the desired film. Photo enhanced CVD uses photon energy in place of or as an adjunct to the thermal energy needed for reactions. CVD is used extensively for plug fill but is not widely accepted for depositing refractory barriers due to a number of reasons including low quality film, inability to find elements that will not react in the gas stream, film formation with high impurity(Carbon) concentration and expensive precursors.

1.3.2 Physical Vapour Deposition(PVD):

In PVD physical processes are used to transform target material into a vapour state which is then transported to the substrate. Evaporation and sputtering are both classified under physical vapour deposition. For evaporation the source solid is heated by resistance, induction or particle beam bombardment to generate the vapour. Sputtering involves ions being accelerated through a potential gradient to bombard the target, where, through momentum transfer atoms near the surface become volatile and leave the surface as a vapour. In these techniques externally induced ionization and/or ion beam bombardment of the substrate can be manipulated to obtain certain desired modifications in the properties of the deposited film[3].

Evaporation:

Evaporation can be used to deposit metal device interconnections and epitaxial films (molecular beam epitaxy). Evaporated films are formed when source material is heated at an elevated temperature so that a large number of atoms or molecules leave the surface of the source and condense on a cooler substrate. The source is heated by either RF induction, electric resistance, or electron bombardment[10]. Evaporation using an Electron-gun is very common for refractory metals such as W, Ti and Mo. Even though it is a simple and cost effective method of producing thin films, the disadvantages outlined below have limited its use in advanced applications.

Advantages and Disadvantages of Evaporation[3]:

ADVANTAGES:

1. High deposition rate,
2. Can be used with most metals,
3. Absence of trapped gases,
4. Equipment required is less expensive,
5. No radiation damage for filament or crucible evaporation.

DISADVANTAGES:

1. Difficult to do compounds because of preferential evaporation rate of one or more of the alloy components.
2. Substrate heating is higher.
3. E - gun evaporation causes radiation damage.
4. Step coverage is poor.
5. Contamination originating from melt holders.
6. Surface cleaning is difficult in the same chamber.

Sputtering:

Sputtering is the most widely used method for metallization. In the sputtering process, energetic positive ions of moderately heavy mass bombard the target material. Argon is generally used because it is an atomic gas which is chemically inert and thus will not react with the target material. Momentum transfer from the bombarding ions causes material to be ejected from the surface of the solid target. The dislodged particles then travel through the plasma to the substrate and form the thin metal film.

The metal target is placed into the vacuum chamber along with the substrate. The chamber is then evacuated to a base pressure of at least 10^{-6} Torr (1 Torr = 133 Pa).

After the base pressure has reached an accepted level, the chamber is backfilled with a working gas until the desired working pressure is reached (typically 9 - 12 milliTorr), at which point a plasma (the source of gas ions for target bombardment) could be started and maintained using an electric discharge. Generally the target is negatively charged using a power supply with typical voltages ranging between -300 to -400V. RF systems can achieve a negative voltage at the target through self-biasing. The substrate serves as an anode (positively charged or ground).

A substantial majority of the particles ejected from the target are single atoms, however, dimers [two atom particles] and multiple atom particles also are constituents of the flux arriving at the substrate surface from the target[11, 12]. The proportion of sputtered clusters to single atoms is dependent on the target material and seems to be below 5% for polycrystalline metal targets[13]. Dimers are more prevalent than clusters containing more than two atoms by an order of magnitude. Researchers have suggested that clusters can be formed by single atoms interacting after they have been dislodged from the target surface and before reaching the substrate as well as being dislodged from the target in a cluster state[14]. For most simulation algorithms sputtered particles are considered to be single atoms.

Sputtering System

Figure 1.4: Diagram of a sputtering system.

1.4 Sputtering Techniques

Fig. 1.4 illustrates a typical sputtering system which can be modified to perform different forms of sputtering. Sputtering techniques are differentiated by details of plasma generation, use of electrons in the plasma, the use of collimators and whether film is being deposited or etched. Plasma is a collection of positively charged, negatively charged and neutral particles[15]. Charge neutrality requires that the number density of positive and negative charges be equal. For film deposition or etching a self-sustaining discharge between cathode and anode must be maintained.

1.4.1 DC Sputtering

Figure 1.5: DC sputtering system.

Figure 1.5 depicts a sputtering system operated by DC current. A breakdown voltage is applied so that Argon gas can be partially converted to plasma. The electron field applied between cathode and anode causes electrons emitted from the cathode to travel toward the anode. The electrons participate in a fixed number of ionizing collisions with neutral atoms during this time causing additional electrons and ions to be generated. The applied field accelerates the new electrons towards the anode and the new ions toward the cathode where, if their energy is large enough, they can

cause the cathode to be sputtered and secondary electrons to be emitted. The plasma glow becomes self-sustaining when the number of secondary electrons produced at the cathode is sufficient to maintain the discharge. The substrate resides at the positive anode which is physically situated opposite the target at the cathode, and intercepts a large proportion of sputtered material from the target.

1.4.2 RF Sputtering

In RF sputtering an alternating voltage is applied between the cathode and anode so that the target can be bombarded by positive ions and then by negative electrons in consecutive and alternating pattern. Unlike DC systems, targets used for RF sputtering can be insulators. If an insulator target is used for DC sputtering, the target will initially be bombarded by positive ions and become positively charged until it repels any further positive ion bombardment. RF sputtering has been widely used for both deposition and cleaning targets and substrates.

1.4.3 Magnetron Sputtering

In magnetron sputtering (Fig. 1.6) a magnet is placed behind the target to create a magnetic field that constrains the movement of secondary electrons to helical paths. For RF and DC sputtering most secondary electrons emitted from the target do not cause ionization of Ar atoms and end up being collected at the anode substrate

Figure 1.6: Schematic of a magnetron sputtering system.

causing unnecessary heating. Sputtering rates are low if electrons pass through the discharge without generating ions. In magnetron sputtering the electrons are confined with respect to their trajectories which enhances the probability of ionizing collisions. Fewer high energy electrons escape from the target region to strike the substrate[16], thus avoiding heating and allowing the substrate to remain essentially at room temperature. The magnetic field restricts the plasma to an area just above the surface of the target resulting in more efficient sputtering. Due to the magnetic confinement a "race track" erosion profile is generated on a target. Deposition rates for magnetron

sputtering are about one order of magnitude higher than for RF sputtering.

1.4.4 Reactive Sputtering

Compound materials can be deposited by reactive sputtering using DC power. Oxides, nitrides and hydrides are produced by introducing oxygen, nitrogen or hydrogen together with the working Argon gas[17]. The sputtered material and gas react to create the deposited compound thin film. In this form of sputtering the ionized active gas molecules combine with the target material to form a metal compound while the inert gas molecules dislodge target atoms.

1.4.5 Bias Sputtering

In bias sputtering the substrate is purposefully biased with a negative potential to attract positive Ar ions and cause resputtering of the growing film. Resputtering is sometimes desired as a means for redistribution of the deposited film to areas such as sidewalls of trenches or vias that do not receive direct deposition by incoming sputtered atoms. Film properties such as step coverage, grain size, resistivity, surface roughness and alloy composition can be controlled through bias sputtering. Deposition rates for this sputtering method are low and ion damage of the films can occur.

1.4.6 Sputter Etching

Sputter etching removes material from the substrate rather than depositing it. A negative voltage is placed at the substrate and the resulting field accelerates argon ions toward the substrate surface. The bombarding argon ions transfer momentum energy to atoms near the surface of the films allowing these atoms to leave the film surface or be redistributed along the topography. Sputter etching can be used to improve step coverage and film density through atomic redistribution. Targets and substrates can be cleaned by having the surface layers removed by sputter etching. This process is known as presputtering.

Patterns can be generated on a surface by selectively etching the surface using a protective mask. The argon ions arrive essentially normal to the surface because the electric field is normal to the target surface. The predominantly normal directional nature of the incoming energetic ions allows substrate surface material to be etched with a high degree of anisotropy (i.e. basically vertical etch profiles are produced). Sometimes, this etching mechanism can be quite non-selective against both the masking material and underlying material to be etched. The selectivity is determined by the sputter yield differences of the materials. Selectivities are generally not adequate because the relative sputter yield between most materials is within a factor of three.

Figure 1.7: Schematic of a collimated sputtering system.

1.4.7 Collimated Sputtering

As contact/via sizes decrease, their aspect ratios (depth:width) become very large, making them difficult to coat with contact, barrier or conducting metal films[18]. Placing grid vanes between the target and the substrate to collimate the sputtered atomic flux before it reaches the substrate has been proposed as a means of enhancing feature coverage[18]. Collimated sputtering(Fig. 1.7) utilizes a physical collimator to control the flux of the sputtered atoms onto the substrate, yet the technique retains most of the advantages of conventional planar magnetron sputtering deposition.

Sputtered atoms with large incident angles generally do not reach the bottom of high aspect ratio vias/contacts and trenches. Collimation suppresses these atoms and allows them to deposit at the bottom of high aspect ratio topography, thus improving overall film coverage.

1.4.8 Long Throw Sputtering

To achieve the same goal long throw sputtering narrows the flux distribution by using a large target-substrate distance and decreased deposition pressure. The working pressures for long throw sputtering can be as low as 1mT. The flux distribution generated at the target remains relatively narrow because scattering is substantially decreased at these low pressures. From simple geometric arguments, the large substrate-target distance eliminates flux atoms with off-normal directions reaching the substrate. The flux distribution reaching the substrate is very narrow which enhances bottom coverage of high aspect features.

1.5 Physics of Sputtering

Deposition sputtering can be segmented into three logical sequences: ion bombardment at the target surface, transport of the sputtered atoms to the substrate or growing film surface and processes involved in film growth.

1.5.1 Target Processes

After a bombarding ion strikes the surface, various phenomena can take place:

1. The ion maybe reflected probably in a neutralized state.
2. Ion implantation can result from the ion being buried deep into the target,
3. The ion impact can cause ejection of a secondary electron,
4. The ion impact may result in the creation of vacancies and interstitials in the target. Major structural rearrangements such as lattice defects can also occur,
5. The ion impact may set in motion a series of collisions between atoms in the target known as a collision cascade, leading to the possible ejection of one of the atoms. This ejection mechanism is called sputtering,
6. Target heating occurs due to inefficient momentum transfer. Ejected atoms leave the target with roughly 1% of the original ion energy.

1.5.2 Sputtered Flux

Specific angular and energy distributions for ejected species best describe the overall cumulative effects of continuous multi-particle bombardment of the target material. Experimental data exists about these distributions and it is generally held that these distributions are roughly “cosine” i.e. random ones. The initial distributions at the

target are then modified through gas scattering as the particles move through the plasma. The resulting angular and energy distributions of sputtered flux striking the substrate surface have a direct and significant effect on the microstructure surface profile and deposition rate of the depositing film. It is extremely useful to have an understanding of these distributions to accurately portray and predict film growth from sputtering. For metal targets, it has been suggested that the angular distribution consists of two parts, randomly ejected particles (cosine distribution) and particles emitted in a closest packed direction. The latter component's direction is reflective of the crystal lattice structure of the target material. Sputter distributions near the target surface are modified through scattering of sputtered particles by argon ions and neutrals in the ambient before reaching the substrate. Thus, working gas pressure must be taken into account when trying to determine the particular shape of the angular distribution at the substrate.

1.5.3 Microstructure Growth and Film Properties

Microstructure growth mechanisms are dependent on the fabrication technique and materials used[19, 20, 21, 22]. Thin film characteristics are determined to a great extent by the intrinsic microstructure of the deposited films. Solid films may be either single crystal, polycrystalline or amorphous. Refractory metal films are generally polycrystalline, and as shown in Fig. 1.8 composed of multiple strands of roughly

Figure 1.8: Microstructure of metal thin films.

cylindrical columns that extend from the substrate to the top of the deposited film surface.

Initially when the atoms arrive at the substrate surface, one of three different events might occur:

1. Atoms reflect off the substrate surface
2. Atoms are adsorbed for a while and later re-evaporate
3. Atoms permanently absorb on the substrate surface

For sputter deposited metallization, the first event is unlikely to occur[1]. Events 2 and 3 create adatoms. Adatoms are atoms which are absorbed at the surface. Adsorption is probable when the binding energy between the adsorbed molecule and the surface is large. An adatom can be in either physisorbed or chemisorbed state. Physisorbed adatoms are not chemically bonded to the substrate surface atoms but are “weakly held” to the surface by very weak forces; the van der Waals or fluctuating dipole forces. In this state, adatoms might diffuse over the substrate surface, be re-emitted into the vapour phase or become chemisorbed.

Figure 1.9: Illustration of film nucleation and growth processes.

Chemisorbed atoms are chemically bonded to the surface lattice structure through “electron sharing”. Adatoms in this final state are part of the lattice. Nucleation occurs when adatoms interact to form chemisorbed aggregates. Film growth can

occur from nucleating sites after the nuclei exceed a certain critical size, above which subsequent cluster growth is energetically favorable. Aggregates of adatoms that fail to exceed the critical size will decompose. This process within the film growth mechanism is called the Nucleation stage. Figure 1.9 is a simple illustration of the process.

There are three basic forms of nucleation which are differentiated by the diffusivity the target atoms have with the substrate and initial layer of film growth. For Frank-van der Merwe[23] nucleation the surface and initial monolayer diffusivity are large resulting in epitaxial growth (Fig. 1.10a). The diffusivity allows continuous atomic layers to be formed. The diffusivity for Volmer-Weber nucleation (Fig. 1.10b) is small thus the initial atomic layer is not continuous but is rather a collection of “islands” of growth. These initial layers of growth will develop, through shadowing and low diffusivity, into the columnar microstructure that is representative of the films analyzed in this thesis. Stranski-Krastanov nucleation (Fig. 1.10c) combines the growth mechanisms present in the other nucleation processes. The diffusivity is large between the substrate and target atoms but is low between the initial monolayer and subsequent target atoms. Thus, the initial monolayer is continuous but subsequent growth is columnar.

During the Nucleation stage, films typically nucleate as separate and individual small islands. These nuclei slowly grow together to eventually form a continuous film

Figure 1.10: (a) Frank-van der Merwe nucleation, (b) Volmer-Weber nucleation and (c) Stranski-Krastanov nucleation.

layer over the substrate while creating perturbations that initiate columnar growth. This initial layer will be the base on which future layers of film will grow. Thus, consecutive surface diffusion mechanisms will be different from those described for the first few monolayers. Once the initial film layers have formed and columnar growth initiated, surface diffusion and geometrical shadowing essentially determine the microstructure and properties of the film. Perturbations in the growing film allow for areas that are relatively higher than others. Geometrical shadowing occurs

when these relatively higher parts intercept a proportionally greater percentage of the incoming flux than neighboring sites and hence grow faster - resulting in shadowing of adjacent film regions entirely and the creation of film columns. Surface diffusion can decrease the effects of shadowing by redistributing material from regions of higher to lower energy. At higher temperatures, grain boundary and bulk diffusion can have a similar effect.

Parameters used to optimize film properties, such as substrate temperature, gas pressure, substrate bias, target-substrate distance etc. will modify the relative importance of shadowing and diffusion during film growth. Figure 1.11[24], illustrates qualitatively the effects on microstructure of gas pressure and substrate temperature.

The deposition temperature has a direct impact on the diffusion process and thus can significantly effect film microstructure. The ratio T/T_m , where T is the deposition temperature of the substrate and T_m is the melting point of the respective material, can be used to make general predictions about film microstructure. At temperatures low relative to the melting point, surface diffusion is not significant and shadowing dominates. This results in zone 1 (Fig. 1.11) film microstructure that is porous, with individual microcrystalline columns separated by open boundaries as a result of geometrical shadowing, low overall density and significant microroughness (Fig. 1.12) due to insufficient surface diffusion.

As the substrate temperature is increased (upto $T/T_m = 0.5$), surface diffusion

Figure 1.11: Structure model.

increases and results in films with broader, more densely packed columns of zone 2. The transition regime between zone 1 and zone 2 films is called zone T and is characterized by a dense array of fibrous columns. If the temperature is increased further, grain boundary diffusion, bulk diffusion and grain growth become the dominant influence on film microstructure development. Columns are replaced by large polycrystals of zone 3 growth.

Film microstructure is also directly affected by the deposition pressure (Fig. 1.11). Higher pressures result in lower adatom energy at the substrate surface because adatom kinetic energy is lost during scattering events with working gas atoms. The

Figure 1.12: Overhead micrograph of thin metal film growth at low T/T_m ratio.

lower adatom energy results in decreased surface diffusion. These films have higher surface microroughness and lower reflectivity like zone 1 films. Scattering events decrease at lower pressures resulting in increased substrate heating and larger surface diffusion lengths. Films deposited at lower pressures have smoother brighter surfaces(zone T structure).

Figure 1.13: Peeling due to stress in thin metal films.

Film stress:

Intrinsic mechanical film stress can cause severe problems in many materials applications, particularly if film adhesion to the substrate is poor, in which case tensile stresses result in peeling and compressive stresses in wrinkling[25]. Fig. 1.13 shows the result of stress on W thin film deposition. Stress also effects important film processes such as diffusion and chemical reactivity, as well as material properties; resistivity, resistance, energy band gap in semiconductors and insulators.

A film is under stress when it is not in thermodynamic equilibrium. Stress can

Figure 1.14: Depictions of films under tensile or compressive stress.

be either compressive or tensile . As shown in Fig. 1.14, tensile stress causes the film to contract with respect to the substrate while compressive film stress creates the opposite effect. The total stress in a film is comprised of thermal stress and the films intrinsic stress.

Thermal Stress:

Thermal stress is caused by the difference in thermal expansion coefficients of the film and substrate material. The stress condition is created/modified by the temperature cycle that the film and substrate couple are subjected to during the fabrication process. Substrate temperature is also increased by energy transfer from bombarding ions during sputter deposition and substrate pre-heating. Thermal stress develops while

the sample cools, i.e. after deposition, annealing or other forms of heat treatment. Thermal stress is proportional to the ratio T/T_m and is a secondary factor to intrinsic stress at low substrate or deposition temperatures. Metals used for this thesis have high melting points and consequently resultant films have negligible thermal stress.

Intrinsic Stress:

Intrinsic stress is a general term to define all other stresses excluding thermal stress.

Intrinsic stress can be caused by one or more of the factors listed below:

1. Substrate and film lattice mismatches,
2. Film microstructure and purity,
3. Film defects,
4. Volume changes caused by chemical or metallurgical interactions,
5. Anisotropic growth,
6. Surface effects such as surface tension.

For polycrystalline films the stress created by lattice mismatches is very small, and the net intrinsic stress is held to be independent of the substrate type or orientation. Intrinsic film stress is a strong function of deposition parameters because they control

most of the stress factors listed above. The most significant deposition parameters for film stress are:

1. Substrate temperature
2. Working gas pressure
3. Deposition rate and energy
4. Substrate bias
5. Vacuum chamber geometry
6. Angle of incidence

Deposition temperature determines the significance of intrinsic stress. Intrinsic stress develops at temperatures under $T_m/3$. Atomic mobilities are large after this temperature point and reduce some of the factors that cause intrinsic stress.

Intrinsic stress strongly depends on the void and impurity content in a film as well as the columnar microstructure. A reduction in porosity can increase tensile stress by reducing the distance between film atoms, thus increasing the force exerted by film atoms separated by voids. Tensile stress decreases significantly when void size and number density are reduced as a film becomes more dense and compact at low pressures and/or due to energetic ion bombardment. Ion bombardment compacts

the growing film and creates a nearly perfect lattice inside grains of the growing film[26].

Chapter 2

Simulation of Thin Film Microstructure and Growth

2.1 Introduction

As feature sizes shrink, knowledge about previously unimportant characteristics (such as density variation and columnar microstructure) will become crucial [27]. Film qualities such as microstructure, surface roughness, film density and surface profile have a direct impact on circuit reliability and performance. As VLSI dimensions decrease and performance requirements increase, these film quality parameters must be analyzed and optimized. VLSI topography simulators are being developed and used for this specific function. Their primary purpose is to provide detailed depictions of films

at various stages of the development process.

Metallization simulations may provide realistic and detailed depictions of metal thin film deposition faster and at lower cost than is possible through experimentation. Experimenters can test ideas using simulation methods at an efficiency not feasible experimentally. Deposition processes consist of very complex multi-parameter physical and/or chemical interactions. Simulation packages can often assist in the fundamental understanding and optimization of these processes. However, the same process complexity requires abstractions and approximations to be made in order to define a functional model. Thus, simulation results can not guarantee realistic depictions and can only be used as a complement and supplement to experimental verification.

A useful metallization simulation package will provide the following capabilities:

1. Simulation of a variety of deposition techniques
2. Representation of arbitrary sub-micron substrate topography
3. Depiction of step coverage and film microstructure
4. Fast and cost effective computer execution

An engineering workstation platform is the best solution to constraints imposed between computing cost and performance. To decrease computational requirements even further, a common approximation is to reduce models from three to two dimen-

sions. This approximation is only valid in situations where there is a symmetry which reduces the dimensions of the problem (trenches, steps or vias).

2.1.1 Modeling Techniques

There are several techniques used in the simulation of thin film growth. The level of detail, approximations used and computational requirements set these models apart. Molecular dynamics[28] models calculate the forces between all participating atoms and solve the equations of motion resulting from these forces. Due to tremendous computational requirements, MD models are not generally used in VLSI topography simulation process tools. Atomistic Monte Carlo models are similar to MD models but assume a greater degree of independence between atoms and make some assumptions about equilibrium conditions. Atomistic models can avoid time scale problems that exist for MD simulations and provide detailed microstructure information. But, even very small ULSI structures require a large number of atoms and the computational requirements still limit the use of Atomistic Monte Carlo models in integrated circuit process simulation.

Macroscopic models employ continuum equations as opposed to the detailed atomistic force equations for microscopic models used in MD simulations. SAMPLE and SPEEDIE are popular string advancement models from the University of California at Berkeley and from Stanford University. The films (Fig. 2.1) are depicted in cross

Figure 2.1: SAMPLE film simulation.

section as a continuous line comprised of line segments, called strings. The strings are advanced based on the calculated flux reaching them. Execution is very quick and film deposition, lithography, etching and thermal processes can be simulated. However, string algorithms provide no information on film microstructure. Because microstructure information is important for predicting ULSI metal film performance, string algorithms are limited models for metallization simulations.

Simulations for this thesis were conducted using the SIMBAD software package which incorporates a ballistic deposition model and SIMSPUD, a Monte Carlo transport model, which simulates the flux arriving at the substrate. SIMBAD's ballistic model is a macroscopic model that incorporates statistical atomistic behaviour dy-

namics. Ballistic deposition is a compromise between very detailed atomistic models and very fast string algorithms. SIMBAD deals with abstract particles that reflect the statistical average of many atoms with similar trajectories and energies. The particles are small enough to provide detailed microstructure information while sufficiently few are needed for film depiction to keep simulation times reasonable. SIMBAD's original ballistic model was developed by Professor M.J. Brett at the University of Alberta[29]. Extended models have been developed by T.J. Smy, R.N. Tait and S.K. Dew to study various film properties while adding simulation capabilities for evaporation, sputtering, CVD, wet etching and plasma etching.

To successfully simulate sputtering, the following sequential processes have to be modeled;

1. Plasma ions striking target
2. Generation of sputtered particles at the target
3. Journey of sputtered particles through plasma to the substrate
4. Diffusion and microstructure growth mechanisms at the substrate

The first two mechanisms are not directly simulated, but are accounted for by the target erosion profile that is entered into SIMSPUD. SIMSPUD models the third process and SIMBAD the fourth.

The characteristics of sputter-deposited films reflect the nature of the flux arriving at the substrate. Very little experimental data is available for angular distributions probably because this information is difficult and tedious to obtain experimentally. It is therefore advantageous to develop models to determine angular distribution patterns. SIMSPUD (SIMulation of SPUtter Distributions) is a software package employing such models to provide angular distribution information for a variety of deposition conditions. SIMSPUD is a vapor-transport model that simulates the three dimensional macroscopic path of the individual atom from its emission at the target, during its travel through the working gas until its arrival at the substrate plane[18]. For each individual atom the position, angle and energy are tracked in order to produce statistics on the corresponding sputter distributions and the angular and energy distributions for particles arriving at the substrate surface. For a set of particular deposition conditions such as target material, target erosion profile, working gas pressure, input power etc., SIMSPUD can provide the resultant angular distribution of the sputtered flux at the substrate. This information can be used to determine relative deposition rates, thickness uniformity across a wafer and in conjunction with SIMBAD, step coverage and microstructure of the metallization layer under various deposition conditions[30]. Throughput, yield, performance, and reliability of metallization films can be determined using the information generated by SIMSPUD.

In order to accurately develop distribution profiles, SIMSPUD must incorporate

the effects on atoms of two events. Initially, atoms must be generated at the target with realistic spatial, angular and energy distributions. SIMSPUD[31] must then account for modifications to these distributions as atoms move from the target to the substrate. To model gas scattering in the second phase, SIMSPUD uses an energy dependent collision cross section with a hard sphere scattering model. This model is necessary at higher energies where scattering can cause substantial energy loss and broadening of angular distributions. At low pressures, flux atoms participate in few scattering events with argon gas and have high energy and relatively unchanged angular distributions at the substrate.

SIMBAD uses the angular distribution from SIMSPUD to simulate atoms hitting the substrate or the growing film. It then models the subsequent movement of an atom until it finally deposits at a certain location. Initially developed for the simulation of sputtered thin films deposited at temperatures which are low with respect to the depositing material's melting point, SIMBAD is a two dimensional model of film growth over nonplanar topography, where the material in the growing film is represented by packed discs. Each disc represents the average behavior of many individual atoms. Thus, the model is in essence a statistical average of the movement and deposition of atoms within the simulation region.

The basic SIMBAD deposition model has been described previously [18, 32, 33, 8, 34]. In the SIMBAD model two-dimensional hard disks are launched with linear tra-

jectories from a random point at the top of the simulation space. Periodic boundary conditions are defined for the lateral edges of the simulation. The disks are launched with an angular distribution for the specific deposition technique and conditions to be simulated. The particles path from an initial random starting point through a determined trajectory to the growing film is traced. It is important to realize that the trajectory of each disk represents the average path of a large number of atoms following a similar trajectory. The disk trajectory is not a reflection of an individual atomic trajectory. As the mean free path for adatoms in the gas phase is very large with respect to the size of the simulation region for typical deposition pressures, these discs move ballistically until they contact the growing film or the substrate. As the disk size is much smaller than any feature of the topography, or the sputtered film, SIMBAD realistically simulates the ballistics of the sputter process[35].

Once at the surface, the final resting spot for the disc is determined by calculating the closest cradle point with the largest coordination number(highest number of nearest neighbors) within a radius of 4 disc diameters from the impact point. Fig. 2.2 graphically illustrates this process.

This relaxation process simulates surface diffusion of the particles which leads to reduction of surface energy consistent with areas of high curvature. This basic algorithm models the nucleation, self-shadowing and columnar growth typical of sputtered refractory metals. It also models, of course, any shadowing caused by features present

Figure 2.2: Basic SIMBAD model using relaxation. Light grey discs indicate potential neighbors in the region of relaxation for a diffusion length of 4.5. Dark grey disc is the final position of depositing disc.

in the substrate, such as a step or via. Fig. 2.3 is a simulation of Tungsten deposition using the standard SIMBAD model.

Figure 2.3: Tungsten thin film simulation using standard SIMBAD model.

Chapter 3

Mushrooming of Refractory Metal Thin Films due to Directed Flux

3.1 Introduction

¹

Refractory metals can be used as an intermediate barrier layer between the Silicon and Aluminum to prevent aluminum penetration[4]. Refractory metal barrier layers for commercial fabrication are deposited primarily using sputtering. For the film to be a good barrier it is imperative that the Tungsten deposition be uniform over the VLSI topography. Fig. 3.1a helps clarify certain definitions used to describe metallization

¹The material in chapters 3 and 4 has been published in the Journal of Applied Physics[36]

processes over VLSI surface geometries. Good step coverage or uniform metallization, especially inside topographical features, is extremely important. Open circuits and electromigration failure can result because of poor step coverage. However, as the aspect ratio is increased it becomes increasingly difficult to obtain uniform coverage. Specifically, the bottom coverage (film coverage at the bottom of a topographical feature) usually decreases as the aspect ratio is increased. Recently, collimators have been used to create highly directional flux that improves step and bottom coverage and increases the effectiveness of barrier layers[37].

However, with the advent of the use of collimators the directional flux produces a significant change in the profile of the deposited film[38] and a similar effect occurs in long throw sputtering. Fig. 3.1a shows a typical deposition profile for a broad adatom flux which would result from a large industrial target. The placement of a collimator between the substrate and the target would filter out the oblique flux and produce an adatom flux that is narrower and primarily in the vertical direction. This alteration of the adatom flux increases the bottom coverage of the film, but new features of the profile arise. A typical deposition profile for a directional sputter flux deposition is shown in Fig. 3.1b. The film exhibits an extended lateral growth from the top corners of the trench. We refer to this type of growth as “mushrooming”. This mushrooming can cause a thick deposition to close the contact opening. The mushrooming also shadows incoming flux and can cause a notch to form in the film coverage just below

the top corners of the contact[38]. Notch formation can result in open circuits of the chip and incomplete barrier or encapsulation protection; deposition results that are highly undesirable and lead to circuit failure.

Figure 3.1: a) Definition of step coverage and bottom coverage of a film deposited over a via. b) Definition of mushrooming angle and notch formation for a film deposited using a highly directional flux.

In Fig. 3.2, two SEM(Scanning Electron Microscope) pictures are shown for two different sputtering targets. The first SEM shows the film coverage produced by a RF(Radio Frequency) diode system with a 5 inch diameter target at a pressure of 11 mT. The uniform erosion and large target of this system produces a fairly broad angular distribution. The second micrograph is from a DC(Direct Current) magnetron system with a 3 inch target at a pressure of 8 mTorr. The race track of this system was approximately 1.5 inches in diameter. Due to the non-uniform erosion of this target and smaller diameter the angular distribution is much narrower. The

unusual features of the film in Fig. 3.1b are clearly evident, and have been observed by others[38]. An abrupt mushrooming profile is observed at the top of the trench, a notch exists in the film coverage just below the top corners. As expected for a narrow distribution, the bottom coverage is improved.

Figure 3.2: Film coverage over a high aspect ratio contact using a) a large target system (a 5 inch diameter RF diode target b) a small target sputter gun(3 inch diameter DC magnetron).

3.2 Stress as a possible driving force for Mushrooming

Initially, substantial investigation and experimentation for this thesis was based on the theory that stress within the growing film was causing preferential growth resulting in the extended lateral features. It was hypothesized that a stress gradient

Figure 3.3: Micrographs of Tungsten deposited at (a) 8mT (b) 9mT (c) 10mT (d) 12mT and (e) 13mT.

might lower the surface energy of the growing film at the corners and thus attract a disproportionate number of the adatoms diffusing along the film surface.

Stress within a growing film is dependent on the specific environment in which

a film is grown and can be measured by studying the changes in the radius of curvature of the substrate after film deposition. A qualitative analysis was done using a profilometer to measure whether films were concave or convex (tensile or compressive stress) after film deposition at specific pressures. Results showed that sputter deposited films in the working environment could be under either tensile or compressive stress based upon the working gas pressure. The transition point was found to be approximately 10mT. Below 10mT working gas pressure, resultant films showed compressive stress and above 10mT films displayed tensile stress. Fig. 3.3 shows a number of films deposited with working gas pressure below and above 10mT.

The films were grown to approximately $1\mu\text{m}$. It is apparent from the film micrographs that the mushrooming phenomena is not dependent on film stress. The basic mushroom structure does not change due to film stress whether compressive or tensile. Fig. 3.5 depicts films grown to only .1, .2 and $.5\mu\text{m}$ at 8 and 14mT. The films all show the same mushrooming structure as seen in the $1\mu\text{m}$ films. This suggests that the fundamental mechanism causing mushrooming is independent of film thickness and is assumed to be present at all phases of film development. A post deposition phenomena was therefore discarded as a possible explanation for the extended lateral growth features of the thin films. This view is also supported by the realization that a substantial volume of material exists outside the vertical profile (Fig. 3.4b) of the trench. It is improbable that a refractory metal film with a standard SIMBAD

Figure 3.4: (a) Standard SIMBAD sputtered metal film profile, (b) Film profile with mushrooming.

profile(Fig. 3.4a) could evolve a mushroom structure after deposition.

The primary difference in the films, as working pressure increases, is the enhanced film growth in the corner notch area created by the mushroom structure and side-wall growth. The 1, .5, and $.2\mu\text{m}$ films(Fig. 3.3, Fig. 3.5) all exhibit the same trend of enhanced film growth in the notch area as deposition pressure is increased. Standard SIMBAD simulations(Fig. 3.6) using models discussed previously failed to realistically depict the mushrooming effect.

This thesis will present a model based on the momentum of the adatoms to explain the profile evolution of sputter films with a highly directional flux. The model will be incorporated into SIMBAD and used in conjunction with SIMSPUD. SIMBAD and SIMSPUD have been used previously to simulate various metallization techniques for a variety of conditions and metals. SIMBAD simulations using the modified model

Figure 3.5: Micrographs of Tungsten deposition at pressures of (a) 8mT to a thickness of $0.1\mu\text{m}$ (b) 8mT to a thickness of $0.5\mu\text{m}$ (c) 14mT to a thickness of $0.2\mu\text{m}$ and (d) 14 mT to a thickness of $0.5\mu\text{m}$.

Figure 3.6: (a) SEM micrograph of Tungsten deposition at 8mT using a small target, (b) SIMBAD simulation using standard version.

will be closely compared to experimental results in order to evaluate the validity of the momentum based model for mushrooming as well as other metallization techniques.

3.3 Modeling

SIMBAD's surface diffusion model simulates surface diffusion of adatoms that reduce the surface energy consistent with areas of high curvature. The extended lateral growth features are inconsistent with microstructure growth that simply minimizes surface energy by surface diffusion. Surface energy minimization is not always the dominant influence on surface diffusion of atoms. The SIMBAD growth model was modified to reflect this new realization.

The simulation of the growth of sputtered refractory metals over VLSI topography has generally assumed that the evolution of the profile is dominated by the self shadowing of the adatom flux by the growing film and the initial topography. The mobility of the adatoms on the surface of the film was assumed to be very small (of the order of $0.1\mu\text{m}$) and to only affect the determination of the column size and the microstructure. The diffusion of the depositing flux on the surface has been assumed to be driven by surface curvature and to be independent of the incident angle and momentum (energy) of the depositing flux. Computer simulation programs based on these assumptions have been quite successful in simulating film growth over a variety of topographies and have incorporated a number effects such as ion bombardment and high temperature substrates[31, 18, 32, 33]. However, the energy distribution of the incident adatom flux includes a substantial portion well above the binding energy of the lattice[39]. Although too low to produce a significant amount of intrinsic resputtering[18], these energetic adatoms could retain a significant portion of the original momentum or generate additional activated surface atoms acquiring this momentum. If a specific part of the film profile is receiving a directional flux at an angle to the surface normal this could result in a biased diffusion of the atomic flux in this region.

3.3.1 Momentum induced biased diffusion

Experimental evidence for the biasing of the surface migration of adatoms during evaporation has been reported[40, 41]. Copper and Chromium were evaporated onto cooled tungsten tips and the depositing material was found to migrate to the backside of the tip. The persistence of the adatom momentum parallel to the surface was given as an explanation for these results.

Van de Waterbeemd and Oosterhout[42] shadowed dust particles on a substrate with oblique incidence deposition of Sn followed by Al_2O_3 to prove that Sn adatoms migrate parallel to the vapor incidence beam. The experiment was done to prove Kambersky et al's[43] finding that oblique incidence should result in a non-symmetric atomic velocity distribution at the substrate with some preferences for the projected direction of the beam.

Abelmann and Lodder have used conservation of atomic momentum parallel to the surface to successfully explain effects observed for evaporation on oblique surfaces. They incorporate a model developed by Hara et al which is based on the principle that the momentum of incident vapor atoms parallel to the film plane causes a deviation of the columnar inclination from the vapor incidence direction toward the film surface[44]. There is, also, evidence from molecular dynamics simulations that, during the formation of thin metal films by cluster deposition, the momentum parallel to the surface is not completely absorbed by the lattice[45, 46].

Figure 3.7: Angular (a) and energy (b) distributions for sputtered tungsten with a large target and a small target.

Sputtering is a process that produces an adatom flux of significantly higher energies than evaporation. In Fig. 3.7 angular and energy distributions determined by the simulator SIMSPUD are given for the two sputter systems: a typical magnetron system using a small 3 inch target with a 1 inch radius erosion profile and a typical diode system using a 5 inch target with uniform erosion profile. If, as the evidence suggests, the surface migration of adatoms deposited by evaporation onto a cooled substrate is affected by the kinetic energy of the incoming species, then the sputtering of metals onto uncooled substrates should show more substantial effects.

In order to model this phenomenon we need to understand the effect atomic momentum will have on the surface diffusion process. When an adatom strikes the surface a portion of its energy is lost to the lattice and the rest is retained as kinetic

energy, which must be dissipated before the adatom can be chemisorbed. Sticking coefficients for sputtered refractory metals are near unity[18] and the adatom does not generally leave the surface after the initial collision. As the adatom migrates on the surface it will interact with the surface and any defects (ledges, steps, islands), scattering off these defects and performing a random walk on the surface. Each scattering occurrence may involve a loss of energy and momentum and the walk will continue until the adatom is incorporated into the lattice[47]. The initial presence of a significant momentum parallel to the surface produces two physically different surface transport mechanisms. Initially a fast collisional momentum transfer is important, however, as the adatom loses energy a standard surface diffusion mechanism dominates. The two mechanisms taken together produce, in effect, a biased diffusion of the adatoms.

A model of the momentum induced bias of mobility requires an angular dependence of this bias on the incident flux direction. To this end, as a simple model we assume that the momentum of the adatom normal to the surface is absorbed completely by the lattice, but that some portion of the momentum parallel to the surface is retained by the adatoms generated by the initial collision. In Fig. 3.8 the relevant angles are shown. The initial momentum of the diffusing adatoms parallel to the local substrate surface is therefore

$$P_{\alpha} = C\sqrt{2mE} \sin \theta \quad (3.1)$$

where C is a proportionality constant, E is the initial energy, θ the angle from the

Figure 3.8: Modification of mobility based on disk momentum.

normal and m the mass of the depositing species. The flux of atoms along the surface will be proportional to the average velocity (P_a/m) of the atoms and the number of adatoms arriving at the surface. For a flux striking a surface at an angle θ , the number of adatoms arriving at the surface is proportional to $\cos \theta$. This results in a flux parallel to the surface of,

$$F_a = F \sin \theta \cos \theta \quad (3.2)$$

Where, F is a proportionality constant.

The momentum and energy of this adatom flux will be absorbed by the lattice during the resultant scattering events and diffusion along the surface. If this effect is averaged for all of the incident adatoms striking a region of the surface it can be

expected that the result will be a biased diffusion in the direction of the average angle of deposition. Although the magnitude of the bias is difficult to determine it will be proportional to the adatom flux. This will result in the bias being proportional to $\sin \theta \cos \theta$. This argument provides the angular dependence for the fast collisional momentum transfer, however, the proportionality constant "F" must be fit to experimental results.

It can be seen that the phenomenon described above will have little effect unless the angle of deposition deviates from the surface normal and also the distribution of adatom flux is fairly narrow. If the distribution is normal to the surface then the effect will cancel itself out with adatoms striking from both sides equally. If the distribution is striking the surface obliquely (Fig. 3.9), the magnitude of the effect will be strongly determined by the width of the distribution and the average angle of incidence. The magnitude of the bias in diffusion would be expected to be of the order of the diffusion length.

It may now be clarified why the profile of the growing film is significantly different for a collimated sputtering system or a system with a small target. For such a system the flux is primarily vertical and in Fig. 3.10 the flux striking the growing film is depicted. For the horizontal surface of the film the adatom momentum has little effect and the diffusion of the adatoms in this region would on average be symmetrical. The flux striking the film deposited on the top corners of the trench, however, has

Figure 3.9: Narrow and wide distributions with the same average angle of incidence.

an angle of incidence of around 45° to the surface normal. The adatom flux striking these regions of the film would therefore have a biased diffusion towards the center of the trench. This biased diffusion would result in the transfer of matter along the film surface towards the middle of the trench. This matter transfer is responsible for the formation of the mushrooming of the film at the trench top corners (Fig. 3.6a).

3.3.2 Computer Modeling

SIMBAD in its original model assumed that an atom would impact with the surface and from the initial impact point would symmetrically search the surface for a site of lowest surface energy. The sites had to be within the atomic diffusion length for that

Figure 3.10: Biasing of diffusion in the region of the trench top corner.

particular material. It was straight forward to modify the SIMBAD diffusion algorithm to allow for a biased diffusion. The magnitude of the bias was determined from the surface normal and the incident angle of the disc using the $\sin \theta \cos \theta$ relationship. A proportionality constant remained to be determined and this was obtained by matching with experimental results.

Chapter 4

Results

In general, SIMBAD has produced high quality metallization simulations for the commonly used deposition techniques and metals. Not only does it produce surface profiles like conventional simulation techniques, SIMBAD also provides additional information of the microstructure and local density variations of the film[18, 32, 33, 8, 34]. In order to validate the momentum induced biased diffusion model a careful comparison was done between the original simple SIMBAD model, the modified momentum model and experimental results. It is necessary to explain both the previous success of SIMBAD and to evaluate the predictive value of the momentum model.

Figure 4.1: SEM picture and simulation for evaporation. Scale bar represents $1.2\mu\text{m}$.

4.1 Experimental Equipment

A three target MRC 8620 sputtering system was used for magnetron and RF thin film deposition. A 5 inch target was used for RF diode sputtering and a 3 inch target was used for magnetron sputtering. Tungsten targets had a purity of 98%. The target to substrate distance was 5.8 cm for the RF system and 9.0 cm for the magnetron system. A system base pressure of 4.8×10^{-6} Torr was reached prior to sputtering. Argon(99.999% purity) was the working gas and experiments were conducted at various pressure. The power used for the systems was 100 watts.

4.2 Basic SIMBAD Results

A situation in which SIMBAD has been very successful in modelling is evaporation. Fig. 4.1 presents the SEM photograph for a $0.8\mu\text{m}$ thick Tungsten film deposited over a high aspect ratio trench using evaporation. Fig. 4.1b shows the corresponding SIMBAD simulation with no momentum shift. The simulation results are quite consistent with the SEM photographs. Both the film profile and the microstructure are matched well by the SIMBAD simulations. Although evaporation produces a highly directional flux perpendicular to the substrate, this result is expected, as the evaporated flux is of very low energy and the momentum transferred to the surface adatoms would be small.

A second deposition system which SIMBAD has previously matched well is a sputter system with a large target and therefore a wide distribution. In this case we would expect the momentum shift to be present, but for it to have little effect on the profile or microstructure of the film, due to the wide distribution. In Fig. 4.2 a micrograph of a film deposited over a trench using the RF diode target and two simulations are presented. The first simulation is with no momentum bias and matches the film well. A simulation including the incorporation of a momentum shift is shown in Fig. 4.2c. Little difference in the two simulated films can be seen and the effect of the momentum shift is small. The standard SIMBAD model successfully simulated systems with wide distributions, long diffusion lengths or resputtering because these

Figure 4.2: (a) SEM picture for broad distribution W deposition (b) simulation using original SIMBAD code, (c) SIMBAD with momentum model (momentum shift of $0.05 \mu\text{m}$). In both simulations scale bar represents $1.2 \mu\text{m}$.

effects mitigate the mushrooming phenomena.

Figure 4.3: (a) SEM micrograph of tungsten deposition at 8mT using small target, (b) SIMBAD simulation with no momentum shift, c) SIMBAD simulation (momentum shift of $0.05\mu\text{m}$). In both simulations scale bar represents $1.2\mu\text{m}$.

4.3 Directed Sputtering

In Fig. 4.3 a film deposited over high aspect ratio trenches at 8 mTorr is shown for a small target sputter system (3 inch diameter magnetron).

The angular distribution for this system is shown in Fig. 4.4 and is quite narrow

Figure 4.4: Angular distribution for sputtered tungsten with a large target and a small target.

and similar to the distribution of a collimated system with a larger target. Thus, the adatom flux for this system is highly directional and also energetic and would be expected to produce mushrooming as can be observed in Fig. 4.3a.

The simulation shown in Fig. 4.3b has no momentum shift present and the surface profile is seen to deviate substantially from that of the SEM specifically at the top corners of the trench. The second simulation has a maximum momentum shift of $0.05\mu\text{m}$ (at $\theta = 45^\circ$) and the match to the SEM is significantly improved. The diffusion length for this simulation was $0.04\mu\text{m}$. An interesting feature of the profile is the presence of a notch in the film growth just under the mushrooming. This notch is due to the shadowing of the incoming atomic flux by the mushrooming of the film

Figure 4.5: Micrographs of Tungsten deposition at pressures of (a) 8mT to a thickness of $0.1\mu\text{m}$ (b) 8mT to a thickness of $0.5\mu\text{m}$ (c) 14mT to a thickness of $0.2\mu\text{m}$ and (d) 14 mT to a thickness of $0.5\mu\text{m}$.

at the corners, and is highly undesirable. In order to determine at what thickness this notch formed, films were deposited at thicknesses of $0.1\mu\text{m}$, $0.2\mu\text{m}$ and $0.5\mu\text{m}$ (Fig. 4.5). It can be seen that the notch is present from the initial growth stage.

The formation of the notch and the mushrooming was investigated as a function of deposition pressure and deposition rate. The mushrooming was found to be substantially independent of these two parameters. However, the slight broadening of

Figure 4.6: a) SEM of tungsten deposition at 14mT using small target, b) SIMBAD simulation (momentum shift of $0.05\mu\text{m}$). In simulation scale bar represents $1.2\mu\text{m}$.

the angular distribution if the pressure was increased was found to fill in the notch at high pressures. A film deposited at 14 mTorr is presented in Fig. 4.6. This film exhibits the mushrooming present in the film deposited at 8 mTorr, but the additional gas scattering has slightly broadened the angular distribution and the notch has not formed as noticeably. The simulation matches the SEM with same momentum shift used for 8 mTorr and predicts the less severe notching.

To further investigate the effect of angular distribution changes to notch formation, Tungsten was deposited on a film surface off center by approximately 10 degrees as shown in figure 4.7. The mushrooming is still apparent yet the notch formation is substantially different on either side of the mushroom structure. An angular shift of approximately 10 degrees caused the notch on the left side to be completely filled in.

Figure 4.7: Micrograph of Tungsten deposition at 8mT with surface off center by approx. 10 degrees.

4.4 Three-dimensional Simulations using Momentum Biasing

Concurrently with the author's research, Dr. Tom Smy and Khalid Sheerger were using the 3-D SIMBAD model to simulate non-uniform and asymmetric film coverage over vias and contacts. The 3-D SIMBAD model has two versions; a quasi 3-D model that assumes cylindrical symmetry and an interpolated model that allows for simulation of systems that are not cylindrically symmetric.

As wafer sizes increase non-uniform and asymmetric film coverage over vias and contacts also increases at the wafer edge. This is due to directional and asymmet-

ric flux reaching the die at the wafer edges. Dr. Tom Smy and M. K. Sheergar[48] deposited films and performed simulations to investigate asymmetric film growth using the 3-dimensional SIMBAD model. The simulation results showed that films deposited over trenches placed directly under the target center developed symmetrically. Figure 4.8 shows SEM and 3-D simulations of deposited on wafers placed at 2.2 cms, 5.0 cms and 8.1 cms from the central axis of the target. These distances correspond to 15° , 30° and 45° off the central axis of the target.

The poor bottom coverage of these films is due to the high aspect ratio of the contacts. The asymmetrical and non-uniform sidewall and trench corner film growth is evident. The asymmetry increases as the wafer distance is increased. Simulation results are very close depictions of the film micrographs and were only achieved after the momentum effect described in this thesis was incorporated into the standard 3-D SIMBAD model. Use of the standard SIMBAD 3-D model resulted in films that did not closely match experimental results.

4.5 Future Problems and Potential Solutions

For VLSI dimensions of 1 and $.8\mu\text{m}$, the notch effect and trench/via closure due to extended lateral growth are evident problems. As VLSI dimensions decrease from .5 to $.1\mu\text{m}$ and aspect ratios increase to 5 or 10, mushrooming will become a dominant factor for determining barrier quality. The current problems caused by mushrooming

Figure 4.8: SEM micrographs of Tungsten films deposited over contacts at a) 15°, b) 30° and c) 45° off the target central axis.

will increase significantly as dimensions decrease: trench/via enclosure will occur faster and more completely resulting in severe notching and significantly decreased sidewall and bottom coverage.

Figure 4.9a displays the problems outlined. The effects of mushrooming must be minimized while sidewall and bottom coverage enhanced for films to be useful. To achieve this, simulations for Tungsten deposition were performed that effectively changed the flux angles reaching the substrate by modifying the topographical geometry. In figure 4.9b, the sidewalls are slightly off-normal to increase flux atom deposition inside the trench. Sidewall and bottom coverage are enhanced but the density is poor. Mushrooming and notching are still serious problems for this film.

To eliminate the effects of mushrooming and notch formation, rounded corners at the trenches were used for simulations in Fig. 4.10. Topographical features are etched into the substrate. Etching is a relatively precise processing step compared to sputtering. It is possible to create topography with the features depicted in Fig. 4.10.

The topographical curvature is slightly different for each film. Sidewall density is poor for these films because the flux arriving inside the trench is primarily vertical or slightly off-normal. The sidewalls are also blocked from receiving flux atoms due to extended lateral growth at the intersection of the sidewalls and curved trench corners which is very evident in Fig. 4.10a. The trench corners are rounded even more for

Figure 4.9: Simulation of Tungsten deposited on topographies without curved corners and resputtering at 8mT using a) vertical sidewalls and b) off-normal sidewalls.

Figure 4.10: Simulation of Tungsten deposited on various topographies with curved corners, off-normal sidewalls but without resputtering at 8mT.

figures 4.10b and c to decrease the mushrooming effect. In Fig. 4.10c the sidewalls are angled further off-normal than for previous films to enhance sidewall and bottom coverage. The bottom coverage for Fig. 4.10c is about 70% of coverage at the trench top. Together, the films indicate that curved corners and off-normal sidewalls are necessary topographical attributes for producing functional films.

Ion bombardment can redistribute material through resputtering and result in more uniform films with higher density on the sidewalls. Ion bombardment is usually accomplished by a negative potential at the substrate. Simulations were done to test the effects of ion bombardment on film density over various topographies (Fig. 4.11 and Fig. 4.12). An ion bombardment model was incorporated into SIMBAD by Smy et al which generates ion disks as well as film disks. The behaviour of ion disks reflects the statistical behaviour of many ions. Physical or empirical models simulate ion bombardment, resputtering of struck film atoms, and/or local film surface relaxation. Studies of planarization[49] using bias sputtering for Tungsten films have been conducted and compared with SIMBAD simulations for the same process. Simulation results closely depict real films and validate the bias sputtering model in SIMBAD.

Figures 4.9 and 4.11 show that for topographies without curved trench corners resputtering results in films with increased closure because film atoms are resputtered from one side of the extended growth to the other. The mushrooming structure changes from a chevron to a right-triangular shape. For these films, side wall coverage

Figure 4.11: Simulation of Tungsten deposited on topographies without curved corners but with resputtering at 8mT using a) vertical sidewalls and b) off-normal sidewalls.

Figure 4.12: Simulation of Tungsten deposited on various topographies with curved corners, off-normal sidewalls and resputtering at 8mT.

is slightly more dense but bottom coverage is poor because film atoms are removed by resputtering.

The simulations with curved corner topographies show that there is an improvement in sidewall density while film around the corners is more uniform. For films with curved corners and resputtering (Fig. 4.12) the bottom coverage thickness is reduced but is still dense and uniform. With decreased VLSI dimensions, modified topographies and ionic resputtering will both play an important role in developing films with good step coverage and uniform density.

Currently T. Smy et al. are investigating the effects of momentum effects on microstructure columnar growth angles. They are also developing MD simulation software to analyze atomic interaction as sputtered atoms reach the growing film. These efforts should yield a greater predictive capability and understanding of the effects and results elaborated upon in this thesis.

Chapter 5

Conclusion

Experimental results have shown that sputter systems with highly directional incident adatom flux produce unexpected growth profiles for films deposited over VLSI topography. These films exhibit a large lateral growth at the top corners of a trench or step. The extended growth results in a chevron structure that intersects with the sidewall coverage to create a notch. Absence of metal coverage at this junction is extremely undesirable and could lead to circuit failure. As deposition pressure is increased, the absence of material at the notch is less pronounced at the expense of bottom coverage.

Mushrooming is independent of deposition pressure and type of stress(tensile or compressive) the film is subject to. The basic mechanism responsible for mushrooming is present from the initial phases of film growth and is not a post deposition

phenomenon. It is also evident that surface energy minimization is not necessarily the determining factor in diffusion processes for refractory thin film growth.

The lateral growth phenomenon is not well understood, and is not predicted by standard growth simulators. This thesis shows that the assumption of biased diffusion of adatoms based on the incident momentum of the adatom flux can be used to correctly predict the film growth.

A model of the biased diffusion was incorporated into the thin film growth simulator SIMBAD. The program was then used to check the validity of the momentum model by close comparison with SEM cross-sections of W films deposited over trenches. The model was also used to explain the previous success of growth simulators for evaporated films and sputter system that produce broad adatom distributions. Enhanced film growth at the notch is explained by a widening of the flux distribution due to scattering as deposition pressure is increased. The effect analyzed in this thesis could have important ramifications due to the current interest in producing directional angular distributions to improve bottom coverage.

Mushrooming will negatively influence film development as dimensions decrease and aspect ratios increase. Topographies with curved trench/via corners can be used to produce films with substantially decreased lateral growth. Off-normal sidewall features enhance sidewall coverage while resputtering from ionic bombardment redistributes material resulting in greater sidewall density but decreased bottom coverage.

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