Text Book:
Silicon VLSI Technology
Fundamentals, Practice and Modeling
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Thin Film Deposition – Introduction

• Many films, made of many different materials are deposited during a standard CMOS process.
  • Epi layer, Si, SiO₂, contact materials, metals
• Requirements or desirable traits for deposition:
  1. Desired composition, low contaminates, good electrical and mechanical properties.
  2. Uniform thickness across wafer, and wafer-to-wafer.
  3. Good step coverage (“conformal coverage”).
  5. Planarized films.
### Roadmap

\[ \text{Aspect ratio} = \text{AR} = \frac{h}{w} \]

<table>
<thead>
<tr>
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</thead>
<tbody>
<tr>
<td>Technology Node (half pitch)</td>
<td>250 nm</td>
<td>180 nm</td>
<td>130 nm</td>
<td>90 nm</td>
<td>65 nm</td>
<td>45 nm</td>
<td>32 nm</td>
<td>22 nm</td>
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<tr>
<td>MPU Printed Gate Length</td>
<td>100 nm</td>
<td>70 nm</td>
<td>53 nm</td>
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<td>25 nm</td>
<td>18 nm</td>
<td>13 nm</td>
<td>10 nm</td>
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<tr>
<td>Min Metal 1 Pitch (nm)</td>
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<td>152</td>
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<td>76</td>
<td>54</td>
<td>42</td>
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<td>Wiring Levels - Logic</td>
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<tr>
<td>Metal 1 Aspect Ratio (Cu)</td>
<td>1.7</td>
<td>1.7</td>
<td>1.8</td>
<td>1.9</td>
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<td>2.0</td>
<td></td>
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<tr>
<td>Contact Aspect Ratio (DRAM)</td>
<td>15</td>
<td>16</td>
<td>&gt;20</td>
<td>&gt;20</td>
<td>&gt;20</td>
<td>&gt;20</td>
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<tr>
<td>STI Trench Aspect Ratio</td>
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<td>5.9</td>
<td>7.9</td>
<td>10.3</td>
<td>14</td>
<td>16.4</td>
<td></td>
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<tr>
<td>Metal Resistivity ((\mu\text{ohm-cm}))</td>
<td>3.3, 2.2</td>
<td>2.2</td>
<td>2.2</td>
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<tr>
<td>Interlevel Dielectric Constant</td>
<td>3.9</td>
<td>3.7</td>
<td>3.7</td>
<td>&lt;2.7</td>
<td>&lt;2.4</td>
<td>&lt;2.1</td>
<td>&lt;1.9</td>
<td>&lt;1.7</td>
<td>&lt;1.7</td>
</tr>
</tbody>
</table>

- Note the aspect ratios and the need for new materials.
- Note also the number of metal layers requiring more deposition steps.
Thin Film Deposition

- Quality – composition, defect density, mechanical and electrical properties
- Uniformity – affect performance (mechanical, electrical)

![Diagram of Thin Film Deposition](image)

- Voids: Trap chemicals lead to cracks (dielectric) large contact resistance and sheet resistance (metallization)
- AR (aspect ratio) = $h/w$ ↑ with ↓ feature size in ICs.

\[
\text{Aspect ratio} = AR = \frac{h}{w}
\]
Examples Thin Film Depositions

Thinning causes metal resistance to increase, generates heat and lead to failure.

**Figure 9-3** SEM images of coverage and filling problems. (a) shows poor step coverage of a TiW/Al/TiW metal stack layer, deposited by sputter deposition, over an oxide step. (b) shows voids in a Chemical Vapor Deposition (CVD) oxide layer for narrow spaces between metal lines. Photos courtesy of VLSI Technology, Inc.
Basic Concepts

Two main deposition methods are used today:
1. Chemical Vapor Deposition (CVD) - APCVD, LPCVD, PECVD, HDPCVD
2. Physical Vapor Deposition (PVD) - evaporation, sputter deposition

Chemical Vapor Deposition (CVD)

AP-CVD - Atmospheric Pressure CVD
- Cold wall reactor
- Heated susceptor

LPCVD - Low Pressure CVD

Atmospheric Pressure Chemical Vapor Deposition

1. Transport of reactants to the deposition region.
2. Transport of reactants from the main gas stream through the boundary layer to the wafer surface.
3. Adsorption of reactants on the wafer surface.
4. Surface reactions, including: chemical decomposition or reaction, surface migration to attachment sites (kinks and ledges); site incorporation; and other surface reactions (emission and redeposition for example).
5. Desorption of byproducts.
6. Transport of byproducts through boundary layer.
7. Transport of byproducts away from the deposition region.
Wafer Surface Region

\( F_1 = \text{diffusion flux of reactant species to the wafer} \)

= mass transfer flux, step 2

\[ F_1 = h_G (C_G - C_S) \]  \hspace{1cm} (4)

where \( h_G \) is the mass transfer coefficient (in cm/sec).

\( F_2 = \text{flux of reactant consumed by the surface reaction} \)

= surface reaction flux, steps 3-5

\[ F_2 = k_s C_S \]  \hspace{1cm} (5)

where \( k_s \) is the surface reaction rate (in cm/sec).

In steady state:

\[ F = F_1 = F_2 \]  \hspace{1cm} (6)

Equating Equations (4) and (5) leads to

\[ C_S = C_G \left(1 + \frac{k_s}{h_G}\right)^{-1} \]  \hspace{1cm} (7)

The growth rate of the film is now given by

\[ v = \frac{F}{N} = \frac{k_s h_G}{k_s + h_G} \frac{C_G}{N} = \frac{k_s h_G}{k_s + h_G} \frac{C_T}{N} Y \]  \hspace{1cm} (8)

where \( N \) is the number of atoms per unit volume in the film (5 x 10^{22} \text{ cm}^{-3} for the case of epitaxial Si deposition) and \( Y \) is the mole fraction (partial pressure/total pressure) of the incorporating species.

\[ Y = \frac{C_G}{C_T} \]  \hspace{1cm} Mole fraction of the incorporating species in the gas phase.
Growth Kinetics - Temperature

\[ v = \frac{F}{N} = \frac{k_s h_G}{k_s + h_G} \frac{C_G}{N} = \frac{k_s h_G}{k_s + h_G} \frac{C_T}{N} Y \]

1. If \( k_s << h_G \), then we have the surface reaction controlled case (fast transport, slow reaction):

\[ v \approx \frac{C_T}{N} k_s Y \]  \hspace{1cm} (9)

2. If \( h_G << k_s \), then we have the mass transfer or gas phase diffusion, controlled case (slow transport, fast reaction):

\[ v \approx \frac{C_T}{N} h_G Y \]  \hspace{1cm} (10)

- The surface term is Arrhenius with \( E_A \) depending on the particular reaction (1.6 eV for single crystal silicon deposition).
- \( h_G \) is \( \approx \) constant (diffusion through boundary layer).
- As an example, Si epitaxial deposition is shown below (at 1 atm. total pressure). Note same \( E_A \) values and \( h_G \approx \) constant. Rate is roughly proportional to (mol. wt.)\(^{-1/2}\).
Experimental Si Deposition

Key points:
- $k_S$ limited deposition is VERY temp sensitive.
- $h_G$ limited deposition is VERY geometry (boundary layer) sensitive.
- Si epi deposition often done at high T to get high quality single crystal growth.
  - $h_G$ controlled.
  - horizontal reactor configuration.
- There is a substrate orioentation effect when growing Si. Fewer surface bonds (e.g. $<111>$) means slower growth rate.
- $h_G$ corresponds to diffusion through a boundary layer of thickness $\delta_S$. 
Boundary Layer – Diffusion to the Surface

Gas moves with the constant velocity U.

Boundary layer (caused by friction) increases along the susceptor, mass transfer coefficient \( h_G \) decreases, gas depletion caused by consumption of the reacting species (concentrations decrease)

Therefore, Growth rate decreases along the chamber
- Use tilted susceptor
- Use T gradient 5-25°C
- Gas injectors along the tube
- Use moving belt

Deposition of alloys DIFFICULT – various reactions, kinetics (species, precursors)
- Use Physical-VD rather than CVD
Doping in CVD for EPITAXY (Intentional and Unintentional)

The dopant sources at the surface go through:
- dissociation of hydride gas
- lattice site incorporation
- burying of dopants by other atoms in the film

Simulation very inaccurate: chamber design etc.

In deposition, the doping,

\[ C \propto P_i \]

for low growth rates

\[ C \propto \frac{P}{v} \]

for high growth rates

T & time of CVD

autodoping

Calculate all distributions (=contributions) to get C(x,t)

\[ C(x,t) = C_2 \text{erfc} \left( \frac{x}{2\sqrt{Dt}} \right) \]

\[ C_{\text{autodoping}} = C S \exp \left( -\frac{x}{L} \right) \]

\[ vt >> \sqrt{Dt} \]

The growth is faster than the diffusion

**Figure 9-11** Autodoping processes in an epitaxial reactor. Illustrated are evaporation from 1, the wafer frontside; 2, the wafer backside or edges; 3, other wafers; and 4, the susceptor.

**Figure 9-12** Dopant profile in a Si epilayer due to outdiffusion and autodoping. (After [9.3].)
Low Pressure Chemical Vapor Deposition (LPCVD)

- Atmospheric pressure systems have major drawbacks:
  - At high $T$, a horizontal configuration must be used (few wafers at a time).
  - At low $T$, the deposition rate goes down and throughput is again low.

- The solution is to operate at low pressure. In the mass transfer limited regime,
  \[ h_G = \frac{D_G}{\delta_S} \]
  But \[ D_G \propto \frac{1}{P_{\text{total}}} \] (12)

- $D_G$ will go up 760 times at 1 torr, while $\delta_S$ increases by about 7 times. Thus $h_G$ will increase by about 100 times.
- Transport of reactants from gas phase to surface through boundary layer is no longer rate limiting.
- Process is more $T$ sensitive, but can use resistance heated, hot-walled system for good control of temperature and can stack wafers.
Plasma-Enhanced CVD

- Plasmas have been used for cutting and etching, but the concept can be applied to any operation.
- For CVD, a plasma can be used to increase the deposition rate in an environment where the temperature of the substrate must not be significantly elevated.
  - Once metals have been applied, the wafer should not be raised above the melting point of the metal. Typical temperatures for dielectric deposition are from 200 to 350 deg. C.
  - Depositing material without significantly affecting the Dt
- Plasma consists of electrons, ionized molecules, neutral molecules, neutral and ionized fragments of broken-up molecules, excited molecules and free radicals.
- In a plasma, additional energy from the plasma constituents is added to the reactant gases, increasing their energy and the effective deposition rate.
- Free radicals are electrically neutral species that have incomplete bonding and are extremely reactive. (e.g. SiO, SiH3, F)
Plasma Enhanced CVD (PECVD)

- Non-thermal energy to enhance processes at lower temperatures.
  - May be required. Al melting point is 660 deg. C.
- The net result from the fragmentation, the free radicals, and the ion bombardment is that the surface processes and deposition occur at much lower temperatures than in non-plasma systems.
High Density Plasma (HDP) CVD

- Newly developed version of PECVD.
- Remote high density plasma with independent RF substrate bias.
- Allows simultaneous deposition and sputtering for better planarization and void-free films (later).
- Mostly used for SiO$_2$ deposition in backend processes.
Physical Vapor Deposition (PVD)

- PVD uses mainly physical processes to produce reactant species in the gas phase and to deposit films.
- In evaporation, source material is heated in high vacuum chamber. ($P < 10^{-5}$ torr).
- Mostly line-of-sight deposition since pressure is low.
- Deposition rate is determined by emitted flux and by geometry of the target and wafer holder.
- Advantages:
  - Little damage
  - Pure layers (high vacuum)
- Disadvantages:
  - Not for low vapor pressure metals
  - No in-situ cleaning
  - Poor step coverage

Advantages:
- Purer – no filaments, only surface of the source melted
- X-rays generated $\rightarrow$ trapped charges in the gate oxides $\rightarrow$ must be annealed
Evaporation

- The evaporation source can be considered either a point source or as a small area surface source (latter is more applicable to most evaporation systems).

- $\Omega$ is the solid angle over which the source emits ($4\pi$ if all directions, $2\pi$ if only upwards); $N$ is the density of the material being deposited.

- The outward flux $F_k^P$ from a point source, is independent of angle, $\theta_i$, while the outward flux from a small area surface source, varies as $\cos(\theta_i)$ or even $\cos(\theta_i)^n$. 

\[
F_k^P = \frac{R_{\text{evap}}}{\Omega \cdot r^2}
\]

\[
v = \frac{R_{\text{evap}}}{\Omega \cdot N \cdot r^2} \cdot \cos \theta_k
\]
Evaporation (2)

- Nonuniform deposition using a linear target
- Relative normalized deposition rate for a point source and a surface source.

- Wafer holders designed to increase uniformity of deposition
- Use spherical holders & rotate them in a planetary configuration

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**Figure 9-17** Deposition rate of evaporated film as a function of position on substrate for point and surface sources. \( \theta_s = \theta_k \) in this configuration for both point and surface sources. (After [9.6].)

**Figure 9-18** Positions of wafers and sources to achieve uniform deposition in evaporation system on all the wafers. Most evaporation sources behave more like a small area surface source and are in that configuration.
Evaporation (3)

- Deviations from ideal point-sources or small-area surface source emissions can occur.
- For a small area surface source, the ideal emission varies as \( \cos(\theta_i) \), referred to as Knudsen-cell-like behavior.
- Further deviation or non-ideal behavior may vary as \( \cos(\theta_i)^n \).

![Diagram](image)

a. Uniform (isotropic) emission from a point source
b. Ideal cosine emission from a small planar surface source. 
\( (n = 1 \text{ in } \cos^n\theta \text{ distribution}) \)
c. Non-ideal, more anisotropic emission from a small planar surface source. 
\( (n > 1 \text{ in } \cos^n\theta \text{ distribution}) \)
Vapor Pressure – Evaporation Rate

- With evaporation:
  - Can evaporate just about any element but.
  - Difficult to evaporate alloys and compounds
  - Step coverage is poor (line of sight and sticking coefficient of Sc≈ 1).

- E-beam and sputtering used instead of PVD

\[ R_{\text{evap}} = 5.83 \times 10^{-2} \cdot A_{\text{source}} \left( \frac{m}{T} \right)^{1/2} \cdot P_e \]

Evaporation rate of common materials in torr

\[ S_c = \frac{F_{\text{reacted}}}{F_{\text{incident}}} \]

\[ S_c = 1 \quad S_c < 1 \]
• Uses plasma to sputter target, dislodging atoms which then deposit on wafers to form film.
• A major IC technique for alloys (Al, W, Ti, silicides, etc.)
• Higher pressures than evaporation (1-100 mtorr vs. < 10^{-5} torr).
• The plasma contains \( \approx \) equal numbers of positive argon ions and electrons as well as neutral argon atoms.
DC Sputter Deposition (2)

- Similar to PECVD

- Ar⁺ ions are accelerated across cathode sheath to the negatively charged cathode, striking that electrode (the “target”) and sputtering off atoms (e.g. Al).

- Most of voltage drop of the system (due to applied DC voltage, $V_c$) occurs over cathode sheath.

- The atoms travel through plasma and deposit on wafers sitting on anode.
DC Sputter Deposition (3)

- Ar\(^+\) ions are accelerated across cathode sheath to the negatively charged cathode, striking that electrode (the “target”) and sputtering off atoms (e.g. Al).
- The atoms travel through plasma and deposit on wafers sitting on anode.
- Rate of sputtering depends on the sputtering yield, Y, defined as the number of atoms or molecules ejected from the target per incident ion.
- Y is a function of the energy and mass of ions, and the target material. It is also a function of incident angle.
• Sputtering targets are generally large and provide a wide range of arrival angles in contrast to a point source.
  
a) Isotropic flux arrival  
  \[ n = 1 \cos^n \theta \]  
b) Anisotropic flux arrival  
  \[ n > 1 \cos^n \theta \]  

• Arrival angle distribution generally described by \( \cos^n \theta \) distribution (the normal component of flux striking the surface determines the deposition or growth rate).
• Size and type of source, system geometry and collisions in gas phase important in arrival angle distribution.
RF Sputter Deposition

- For DC sputtering, target electrode is conducting.
- To sputter dielectric materials use RF power source.

• Due to slower mobility of ions vs. electrons, the plasma biases positively with respect to both electrodes. (DC current = zero.) \[ \because \text{continuous sputtering.} \]

• When the electrode areas are not equal, the field must be higher at the smaller electrode (higher current density), to maintain overall current continuity

\[ \frac{V_1}{V_2} = \left( \frac{A_2}{A_1} \right)^m \]  

(m = 1-2 experimentally) (13)

• Thus by making the target electrode smaller, sputtering occurs "only" on the target. Wafer electrode can also be connected to chamber walls, further increasing \( V_2/V_1 \).
Ionized Sputter Deposition or HDP Sputtering

• In some systems the depositing atoms themselves are ionized. An RF coil around the plasma induces collisions in the plasma creating the ions.

• This provides a narrow distribution of arrival angles which may be useful when filling or coating the bottom of deep contact hole.
### Table 9-1 Common deposition methods for thin films in integrated circuit fabrication

<table>
<thead>
<tr>
<th>Thin Film</th>
<th>Equipment</th>
<th>Typical Reactions</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Epitaxial silicon</td>
<td>LPCVD, APCVD</td>
<td>SiH₄ → Si + 2H₂&lt;br&gt;SiCl₄ + 2H₂ → Si + 4HCl&lt;br&gt;Also SiHCl₄, SiH₄Cl₂</td>
<td>1000-1250°C&lt;br&gt;Reduce pressure for lower-temperature deposition.</td>
</tr>
<tr>
<td>Polysilicon</td>
<td>LPCVD</td>
<td>Same as epitaxial Si</td>
<td>575-650°C&lt;br&gt;Grain structure depends on deposition conditions and doping.</td>
</tr>
<tr>
<td>Si₃N₄</td>
<td>LPCVD, PECVD</td>
<td>3SiH₄ + NH₃ → Si₃N₄ + 12H₂</td>
<td>650-800°C for oxidation mask.&lt;br&gt;200-400°C (PEVD) for passivation.</td>
</tr>
<tr>
<td>SiO₂</td>
<td>LPCVD, PECVD</td>
<td>SiH₄ + O₂ → SiO₂ + 2H₂&lt;br&gt;Si(OH)₂ (→ SiO₂) → SiO₂ + byproducts</td>
<td>200-800°C&lt;br&gt;200-500°C (LTO)—may require high T anneal.&lt;br&gt;25-400°C (TEOS-ozone, PECVD, HDPCVD).</td>
</tr>
<tr>
<td>Ti and Ti-W</td>
<td>Magnetron sputter deposition (standard, ionized, or collimated)</td>
<td>CVD difficult.&lt;br&gt;Nitrogen can be added to Ti-W to stuff grain boundaries.</td>
<td></td>
</tr>
<tr>
<td>W</td>
<td>LPCVD</td>
<td>2WF₆ + 3SiH₄ → 2W + 3SiF₄ + 6H₂&lt;br&gt;WF₆ + 3H₂ → W + 6HF</td>
<td>250-500°C.&lt;br&gt;Blanket deposition with two-step process using both reactions is common.</td>
</tr>
<tr>
<td>TiS₅</td>
<td>Sputter and surface reaction&lt;br&gt;Conspattering or CVD</td>
<td>Ti(sputtered) + Si(exposed) → TiS₅&lt;br&gt;Sputter/reaction gives self-aligned silicide.</td>
<td></td>
</tr>
<tr>
<td>TiN</td>
<td>Reactive sputter deposition&lt;br&gt;CVD</td>
<td>Ti + N₂ (in plasma) → TiN&lt;br&gt;Organometallic source possible for MOCVD deposition.</td>
<td></td>
</tr>
<tr>
<td>Cu</td>
<td>Electroplating, electroles, sputtering, CVD</td>
<td>Cu²⁺ + 2e⁻ → Cu&lt;br&gt;Electroplating is most common method today.</td>
<td></td>
</tr>
</tbody>
</table>
Manufacturing Methods

• Epitaxial Silicon Deposition
  – Requires access to crystalline surface, or else amorphous Si (a-Si)
  or polycrystalline Si will result
  – CVD of silane or silicon tetrachloride
    • APCVD or LPVD

• Polycrystalline Silicon Deposition
  – Deposited on arbitrary surfaces
  – Sputtered or CVD with less restrictive conditions that epi
  – TEM of grain structure and resistivity follow
Polycrystalline Silicon

a) Undoped thin grains in columns

b) Phosphorous doped with larger grains

c) Undoped and annealed showing little grain grown with annealing

d) Phosphorous doped and annealed showing grain growth with annealing

Figure 9-32 TEM cross sections of CVD polycrystalline films deposited at 625°C: (a) as-deposited, undoped film, showing the thin grains in a columnar structure; (b) as-deposited phosphorus-doped film, showing much larger grain size; (c) annealed (1000°C), undoped film, showing little grain growth as compared to (a); (d) annealed (1000°C), phosphorus-doped film, showing evidence of grain growth as compared to (b). Reprinted with permission of the Electrochemical Society [9.19].
Polycrystalline Silicon Conductivity

- Due to the low resistivity when doped, “poly” has been used both as a gate for MOS transistors and a conductor.
Manufacturing Methods (2)

- **Silicon Nitride Deposition**
  - Films used as a mask against oxidation or as a final passivation layer. A good barrier to water and sodium diffusion.
  - Generally not used in direct contact with silicon due to poor interface properties.
  - LPCVD or PECVD

- **Silicon Dioxide Deposition**
  - Low temperature CVD for dielectric isolation, separating conductive layers. Therefore LPCVD and PECVD typical.
  - HDP CVD also being used
Manufacturing Methods (3)

• Al Deposition
  – A main interconnect material (being replaced by copper)
  – DC magnetron sputtering

• Titanium (Ti) and Titanium-Tungsten (Ti-W)
  – An underlay for contacts and vias between interconnect layers.
  – Typically deposited by sputtering

• Tungsten
  – Contact or via conductor, tungsten via plugs are common
  – CVD using hot-wall and low pressure

• TiSi$_2$ and WSi$_2$ Deposition
  – Silicides of titanium and tungsten. Used to reduce resistivity of polysilicon lines and lower contact resistances with doped N and P regions.
  – Sputtering, co-sputtering, co-evaporation or CVD
Manufacturing Methods (4)

• TiN Deposition
  – Barrier layer in contacts and as an under layer and antireflective layer in interconnects. A very hard metal that can be highly stressed but is brittle.
  – Sputtered using reactive sputtering techniques or CVD

• Copper Deposition
  – The most recent interconnect metal – lower resistivity and less electromigration than Aluminum.
  – PVD by both sputtering and evaporation. CVD possible. Electrolytic plating or electroless deposition
Models and Simulation

- Within the past decade, a number of simulation tools have been developed for topography simulation.

- Generalized picture of fluxes involved in deposition. (No gas phase boundary layer is included, so this picture doesn't fully model APCVD.)

- Essentially the same picture will be used for etching simulation (in Chapter 10).

\[
F_{net}^i = F_{direct(ion)}^i + F_{direct(neutral)}^i + F_{redep}^i + F_{diff.in}^i
- F_{emitted}^i - F_{sputtered}^i - F_{diff.out}^i
\]

- To simulate these processes, we need mathematical descriptions of the various fluxes.
- Modeling specific systems involves figuring out which of these fluxes needs to be included.
- Stanford Profile Emulator for Etching and Deposition in IC Engineering (SPEEDIE) used in text for material.
Considering Incoming Fluxes: Direct

- Direct fluxes are generally modeled with an arrival angle distribution just above the wafer (doesn't model equipment).

\[ F_{\text{direct (neutrals)}} + F_{\text{direct (ions)}} \]

\[ F_{\text{direct}}(\theta) = F^o \cos^n \theta \]

- The \( F_{\text{direct}} \) is the normal component of the incoming flux (which is what is needed in determining the growth rate).
  - Higher pressure systems \( \Rightarrow \) more gas phase collisions, shorter mean free path \( \Rightarrow n = 1 \) (isotropic arrival).
  - Lower pressure systems \( \Rightarrow \) fewer gas phase collisions, longer mean free path \( \Rightarrow n > 1 \) (anisotropic arrival).
  - Ionic species in biased systems \( \Rightarrow \) directed arrival \( \Rightarrow n > 1 \) (anisotropic arrival).
Considering Incoming Fluxes: Viewing Angle

- Once the direct fluxes are known, surface topography must be considered.
- Surface orientation, viewing angle and shadowing are important. Gas phase collisions are neglected near the wafer surface.
Indirect Fluxes

- The indirect fluxes are associated with processes on the wafer surface.

- Surface diffusion is driven by the local curvature of the surface (to minimize the surface free energy) and is given by

\[
F_{\text{diff.in}} - F_{\text{diff.out}} = F_{\text{diff.net}} = \frac{D_s}{kT} \cdot \gamma_s \cdot \Omega \cdot \nu \cdot \frac{\partial^2 K}{\partial S^2}
\]

where \(D_s\) is the surface diffusivity, \(\gamma_s\) is the surface energy, \(K\) is the curvature and \(\Omega\) and \(\nu\) are constants.
Surface Diffusion

- Surface diffusion helps to fill in holes, and produces more planar depositions because molecules can diffuse to "smooth out" the topography.

![Diagram showing high and low sticking coefficients](image)

- \( F^i_{\text{emitted}} \) arises because not all molecules "stick" when they arrive at the surface.

\[
F^i_{\text{emitted}} = (1 - S_c) \cdot F^i_{\text{incident}}
\]  

(17)

where \( S_c \) is the sticking coefficient.

\[
S_c = \frac{F_{\text{reacted}}}{F_{\text{incident}}}
\]  

(18)

- Generally ions are assumed to stick \((S_c = 1)\), neutrals have \(S_c < 1\) and are assumed to be emitted with a cosine angle distribution (no memory of arrival angle).
Redeposited (emitted) Flux

- $F_{\text{redep}(\text{emitted})}^i$ arises because the emitted flux $F_{\text{emitted}}^i$ can land elsewhere on the surface. Thus

$$F_{\text{redep}(\text{emitted})}^{ik} = g^{ik} * F_{\text{emitted}}^k = g^{ik} * (1 - S_c) * F^k$$

(19)

- The redeposited flux at point $i$ due to an emitted flux at point $k$ can then be summed over all $i$ and $k$. $g^{ik}$ accounts for the geometry between $i$ and $k$.

- Thus a low $S_c < 1$ can produce more conformal coverage because of emission/redeposition (usually more important than surface diffusion in CVD).
Sputtered Flux and Ion Flux

- The sputtered flux is caused primarily by energetic incoming ions.

\[ F_{\text{sputtered}}^i = Y \left( F_{\text{argon}}^i + F_{\text{direct(ions)}}^i \right) = Y \cdot F_{\text{ions}}^i \]

where \( Y \) is the sputtering yield. \hspace{1cm} (20)

- \( Y \) is angle sensitive which can be used to achieve more planar surfaces during deposition (example later).

- The sputtered molecules can be redeposited. This is modeled as in Eqn. (19), i.e.

\[ F_{\text{redepos}}^{ik} = g^{ik} \cdot F_{\text{sputtered}}^k = g^{ik} \cdot Y \cdot F_{\text{ions}}^k \]

\hspace{1cm} (21)

- Finally, ions striking the surface can sometime enhance the deposition rate (by supplying the energy to drive chemical reactions for example), so that

\[ F_{\text{ion-induced}}^i = K_i Z^2 \cdot F_{\text{ions}}^i \]

\hspace{1cm} (22)
Models for Different Types of Deposition Systems

- Only the typically fluxes associated with each deposition method are used in simulation.


Stanford Profile Emulator for Etching and Deposition in IC Engineering (SPEEDIE)

The etch and deposition simulator SPEEDIE [2] is intended to simulate two dimensional profile evolution during etching and deposition in gaseous systems. By two dimensional evolution we mean structures that can be represented by a 2D representation either because they are cylindrically symmetric or because one of their dimensions is "infinitely long," i.e., holes (vias) or long trenches. Note that 3D particle movement is considered. The etching part of SPEEDIE is based on a previously reported etch simulator [1][6], that was completely rewritten and numerous additions were added. SPEEDIE predicts time evolution of etch profiles using physical models and parameters extracted from special test structures. The models in SPEEDIE assume:

- Etch and deposition reactor pressure is below a few Torr, such that gas phase collisions within the topological features can be ignored because the mean free path is very large in comparison with the characteristic geometrical dimension of IC devices.
- The fluxes for three types of species are calculated: ions, chemical radicals, and deposition precursors.
- Multiple transport mechanisms that are modeled include direct gas phase fluxes (1), neutral adsorption/re-emission (3), ion induced redeposition (6), surface diffusion (2), and ion reflection.
LPCVD Deposition Systems

In these systems there are no ions involved and hence no sputtering. Surface diffusion also is usually not important.
LPCVD Deposition Systems (2)

- The sticking coefficient $S_C$ is small in these systems so there will be significant desorbed (emitted) and redeposited fluxes.
- Thus at each point on the surface,

$$F_{\text{net}}^i = F_{\text{direct (neutrals)}}^i + F_{\text{redep (emitted)}}^i - (1 - S_C) \left( F_{\text{direct (neutrals)}}^i + F_{\text{redep (emitted)}}^i \right)$$

$$= S_C \left( F_{\text{direct (neutrals)}}^i + F_{\text{redep (emitted)}}^i \right)$$

$$= S_C \left( F_{\text{direct (neutrals)}}^i + g^{ik} (1 - S_C) F^k \right)$$

(23)

- We define $\left( F_{\text{direct (neutrals)}}^i + F_{\text{redep (emitted)}}^i \right) = F_d$

the deposition flux at each point, so the deposition rate is simply given as:

$$\text{Rate} = S_C F_d / N$$

(24)

where $N$ is the film density.

- $\cos^n \theta$ distribution is used for the incoming molecules.
PECVD Deposition Systems

• In these systems an ion flux can enhance the deposition rate by changing the surface reactions. Sputtering is usually not significant because the ion energy is low, nor is direct deposition of ions significant.

\[
\begin{align*}
F^i_{\text{direct(neutrals)}} & \quad \text{Yes} \\
F^i_{\text{direct(ions)}} & \quad \text{No} \\
F^i_{\text{diff (net)}} = F^i_{\text{diff (in)}} - F^i_{\text{diff (out)}} & \quad \text{No} \\
F^i_{\text{emitted}} & \quad \text{Yes} \\
F^i_{\text{redep(emitted)}} & \quad \text{Yes} \\
F^i_{\text{sputtered}} & \quad \text{No} \\
F^i_{\text{redep(sputtered)}} & \quad \text{No} \\
F^i_{\text{ion–induced}} & \quad \text{Yes}
\end{align*}
\]

• Thus

\[
\text{rate} = \frac{(S_c K_d F_d) + (K_i F_i)}{N}
\]  \hspace{1cm} (25)

where \( K_d \) and \( K_i \) are relative rate constants for the neutral and ion-enhanced components respectively.
PVD Deposition Systems

- Standard PVD systems might include DC and RF sputtering systems and evaporation systems.

- Ions generally do not play a significant role in these systems, so modeling is similar to LPCVD systems.

Thus

\[ \text{rate} = \frac{S_c F_d}{N} \]  \hspace{1cm} (26)

- The values for \( S_c \) and \( F_d \) would be different for LPCVD and PVD systems however.

- Sometimes these systems are operated at high temperatures, so a surface diffusion term must be added.

\[ \text{rate} = \frac{S_c F_d + D_s \gamma_s \Omega \frac{\partial^2 K}{\partial s^2}}{N} \]  \hspace{1cm} (27)
Ionized PVD Deposition Systems

- These systems are complex to model because both ions and neutrals play a role.
- They are often used for metal deposition so that Ar\(^+\) ions in addition to Al\(^+\) or Ti\(^+\) ions may be present.
- Thus almost all the possible terms are included

\[
\begin{align*}
F^i_{\text{direct(neutrals)}} & \quad \text{Yes} \\
F^i_{\text{direct(ions)}} & \quad \text{Yes} \\
F^i_{\text{diff(net)}} = F^i_{\text{diff(in)}} - F^i_{\text{diff(out)}} & \quad \text{No} \\
F^i_{\text{emitted}} & \quad \text{Yes} \\
F^i_{\text{redep(emitted)}} & \quad \text{Yes} \\
F^i_{\text{sputtered}} & \quad \text{Yes} \\
F^i_{\text{redep(sputtered)}} & \quad \text{Yes} \\
F^i_{\text{ion-induced}} & \quad \text{Yes}
\end{align*}
\]

\[
\text{rate} = \frac{\left(S_c F_d \right) + F_i - \left(K_{sp} Y F_i \right) + \left(K_{rd} F_{rd} \right)}{N}
\]

where \( F_d \) includes the direct and redeposited (emitted) neutral fluxes, \( F_i \) includes the direct and ion-induced fluxes associated with the ions, and \( F_{rd} \) models redeposition due to sputtering.
High Density Plasma CVD Deposition Systems

- Very similar to IPVD (except neutral direct flux not as important):

\[
\text{rate} = \frac{(K_i F_i) - (K_{sp} Y F_i) + (K_{rd} F_{rd})}{N} \quad (29)
\]
Parameter Values for Specific Systems

<table>
<thead>
<tr>
<th></th>
<th>n (exponent in cosine arrival angle distribution)</th>
<th>$S_c$ (sticking coefficient)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sputter deposition</td>
<td></td>
<td></td>
</tr>
<tr>
<td>-standard</td>
<td>$\sim 1 - 4$</td>
<td>$\sim 1$</td>
</tr>
<tr>
<td>-ionized or collimated</td>
<td>$8 - 80$</td>
<td>$\sim 1$</td>
</tr>
<tr>
<td>Evaporation</td>
<td>$3 - 80$</td>
<td>$\sim 1$</td>
</tr>
<tr>
<td>LPCVD silicon dioxide</td>
<td></td>
<td></td>
</tr>
<tr>
<td>-silane</td>
<td>1</td>
<td>0.2 - 0.4</td>
</tr>
<tr>
<td>-TEOS</td>
<td>1</td>
<td>0.05 - 0.1</td>
</tr>
<tr>
<td>LPCVD tungsten</td>
<td>1</td>
<td>0.01 or less</td>
</tr>
<tr>
<td>LPCVD polysilicon</td>
<td>1</td>
<td>0.001 or less</td>
</tr>
</tbody>
</table>

- **PVD systems** - more vertical arrival angle distribution
  (low pressure line of sight or $\varepsilon$ field driven ions). $\vdash \ n > 1$ typically.
- **CVD systems** provide isotropic arrival angle distributions
  (higher pressure, gas phase collisions, mostly neutral molecules). $\vdash \ n \approx 1$ typically.
- **PVD systems** usually provide $S_c$ of 1. Little surface chemistry involved. Atoms arrive and stick.
- **CVD systems** involve surface chemistry and $S_c <<1$.
  Molecules often reemit and redeposit elsewhere before reacting.
  
  Therefore, CVD systems provide more conformal deposition.
Models in SPEEDIE

LPCVD:

\[
\text{rate} = \frac{S_c F_d}{\text{density}} \left( F_d = F_{\text{direct(neutrals)}} + F_{\text{redep(emit)}} \right)
\]

PECVD:

\[
\text{rate} = \frac{(S_c K_d F_d) + (K_i F_i)}{\text{density}} \quad (F_i = F_{\text{ions}})
\]

Standard PVD:

\[
\text{rate} = \frac{S_c F_d}{\text{density}}
\]

High T PVD:

\[
\text{rate} = \frac{S_c F_d + \frac{D_s}{kT} \gamma_s \Omega_s \frac{\partial^2 K}{\partial s^2}}{\text{density}}
\]

Ionized PVD:

\[
\text{rate} = \frac{(S_c F_d) + F_i - (K_{sp} Y F_i) + (K_{rd} F_{rd})}{\text{density}}
\]

HDP CVD:

\[
\text{rate} = \frac{(S_c K_i F_i) - (K_{sp} Y F_i) + (K_{rd} F_{rd})}{\text{density}}
\]
Calibration of Models - Example: SPEEDIE

Overhang test structure allows calibration of different components

(1) CVD component
(2) Ion-induced deposition
(3) Sputtering with angle-dependent sputter yield
(4) Redeposition
(5) Backscattered deposition
BY OBSERVING DEPOSITION PROFILES IN THE CAVITY CONCLUSIONS CAN BE DRAWN ABOUT THE DEPOSITION MECHANISMS

* INFLUENCE OF CAVITY HIGHT ON DEPOSITION ON THE UNDERSIDE
* TAPERING OF THICKNESS ON TOP SURFACE


J.P. McVittie, “Test Structure and Modeling Studies of Deposition and Etch Mechanisms”,
Talk TC1-WeM6, AVS mtg in Orlando, Florida, 1993
Topography Simulation 1 (Using SPEEDIE)

- SPEEDIE simulations for LPCVD deposition of SiO₂ with $S_c = 1$ (which is more typical of PVD than LPCVD) and varying values of $n$, the arrival angle distribution factor: (a) $n=1$; (c) $n=10$.
- Worse step coverage results as $n$ increases (the arrival angle distribution narrows).
- Even for $n = 1$, conformal coverage is not achieved.

- SPEEDIE simulations for LPCVD deposition of SiO₂ in a narrow trench with the same isotropic arrival angle distribution ($n=1$) but different values of $S_c$: (a) $S_c = 1$; (b) $S_c = 0.1$; and (c) $S_c = 0.01$.
- Reducing $S_c$ is much more effective than changing $n$ if conformal deposition is desired.
Topography Simulation 2 (Using SPEEDIE)

- Results of SPEEDIE LPCVD simulations with the sidewall angle changed. $S_c = 0.2$ and $n = 1$. Note the improved trench filling.

- SPEEDIE simulations comparing LPCVD and HDPCVD depositions.
  (a) LPCVD deposition of $\text{SiO}_2$ over rectangular line. $S_c = 0.1$ and $n=1$.
  (b) HDPCVD deposition, with directed ionic flux and angle-dependent sputtering, over rectangular line showing much more planar topography.

- CMP might still be required in the HDPCVD case to fully planarize the surface.
Topography Simulation 3 (Using SPEEDIE)

- SPEEDIE simulations comparing LPCVD and HDPCVD depositions.
  (c) LPCVD deposition in trench, showing void formation. $S_c = 0.2$ and $n = 1$.
  (d) HDPCVD deposition in trench, showing much better filling.
- HDPCVD has a strong directed ion component and any overhangs that form are sputtered away.

- Actual SEM images of HDP oxide deposition.
Summary of Key Ideas

• Thin film deposition is a key technology in modern IC fabrication.
• Topography coverage issues and filling issues are very important, especially as geometries continue to decrease.
• CVD and PVD are the two principal deposition techniques.
• CVD systems generally operate at elevated temperatures and depend on chemical reactions.
• In general either mass transport of reactants to the surface or surface reactions can limit the deposition rate in CVD systems.
• In low pressure CVD systems, mass transport is usually not rate limiting.
• However even in low pressure systems, shadowing by surface topography can be important.
• In PVD systems arrival angle distribution is very important in determining surface coverage. Shadowing can be very important.
• A wide variety of systems are used in manufacturing for depositing specific thin films.
• Advanced simulation tools are becoming available, which are very useful in predicting topographic issues.
• Generally these simulators are based on physical models of mass transport and surface reactions and utilize parameters like arrival angle and sticking coefficients from direct and indirect fluxes to model local deposition rates.
Additional Notes and Simulations

• Prof. Krishna C. Saraswat, Stanford EE 311
  – http://www.stanford.edu/class/ee311/
  – See Handout 15 Deposition and Planarization Technology

• Prof. Yosi Shacham, Tel-Aviv University
  – http://www.eng.tau.ac.il/~yosish/courses/vlsi1/
  – I 9 vacuu,.pdf
  – I 10 cvd.pdf

• Dr. A. Doolittle, Georgia Tech ECE 6450
  – http://users.ece.gatech.edu/~alan/index_files/ECE6450lecture.htm
  – Lecture 12
  – Klecture 13 & 14