EE C245 – ME C218
Introduction to MEMS Design
Fall 2009

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Lecture Module 3: Oxidation & Film Deposition

Lecture Outline

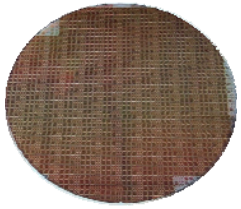
- Reading: Senturia, Chpt. 3; Jaeger, Chpt. 2, 3, 6
  - Example MEMS fabrication processes
  - Oxidation
  - Film Deposition
    - Evaporation
    - Sputter deposition
    - Chemical vapor deposition (CVD)
    - Plasma enhanced chemical vapor deposition (PECVD)
    - Epitaxy
    - Atomic layer deposition (ALD)
    - Electroplating

MEMS Fabrication

Making Mechanical Devices

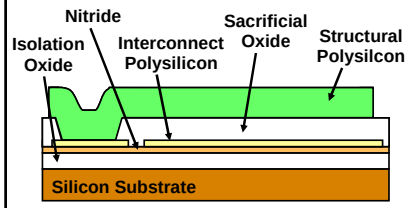
- How best does one make a mechanical product?
- Assembly line production?
  - Pick and place parts
  - Used for many macroscopic mechanical products
  - Robotic automation greatly reduces cost
- *Problem*: difficult to do this with MEMS-scale parts (but not impossible, as we'll soon see …)
- *Solution*: borrow from integrated circuit (IC) transistor technology
  - Use monolithic wafer-level fabrication methods
  - Harness IC's batch methods, where multiple devices are achieved all at once

Automobile Assembly Line

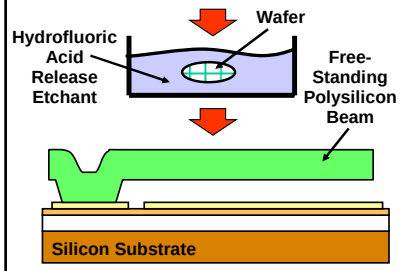


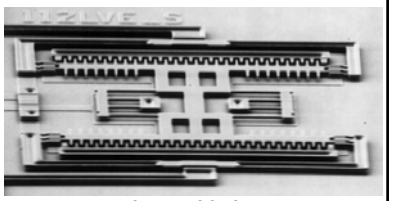
CMOS Integrated Circuit Wafer

Polysilicon Surface-Micromachining



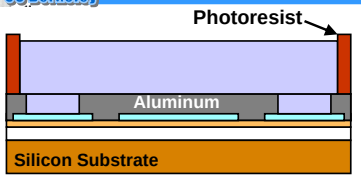
- Uses IC fabrication instrumentation exclusively
- *Variations*: sacrificial layer thickness, fine- vs. large-grained polysilicon, *in situ* vs. $POCl_3$-doping



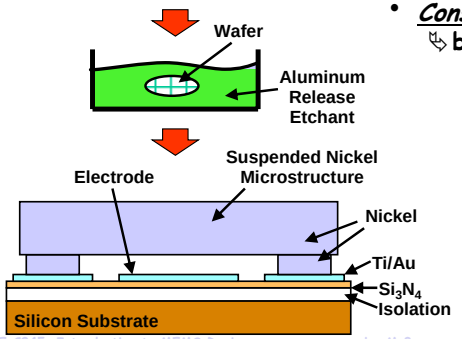


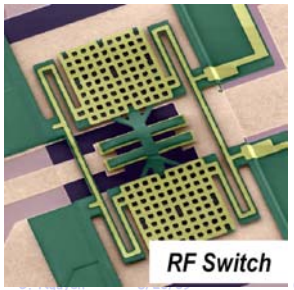
300 kHz Folded-Beam Micromechanical Resonator

Electroplating: Metal MEMS



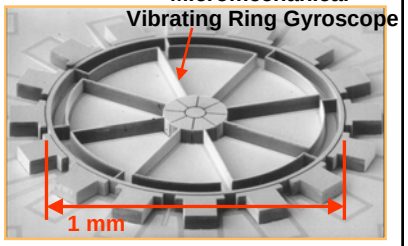
- Use electroplating to obtain metal μstructures
- When thick: call it "LIGA"
- *Pros*: fast low temp deposition, very conductive
- *Cons*: drift, low mech. *Q*
  - but may be solvable?



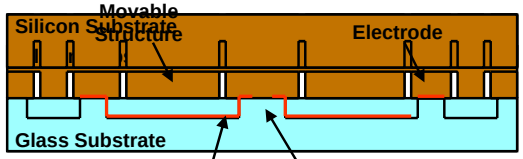


Bulk Micromachining and Bonding

- Use the wafer itself as the structural material
- *Adv*: very large aspect ratios, thick structures
- *Example*: deep etching and wafer bonding



[Najafi, Michigan]



Microrotor (for a microengine)

Oxidation

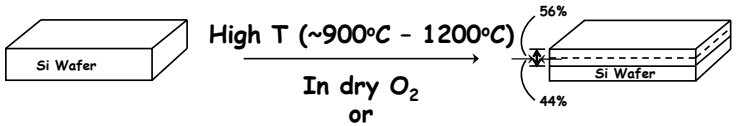
Thermal Oxidation of Silicon

- Achieved by heating the silicon wafer to a high temperature (~900°C to 1200°C) in an atmosphere containing pure oxygen or water vapor
- Enabling reactions:

For dry oxygen: $Si + O_2 \rightarrow SiO_2$

For water vapor: $Si + 2H_2O \rightarrow SiO_2 + 2H_2$

Schematically:

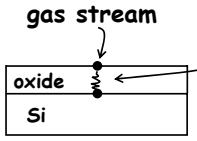


Oxidation Modeling

(1) Initially: (no oxide @ surface)

↳ Growth rate determined by reaction rate @ the surface

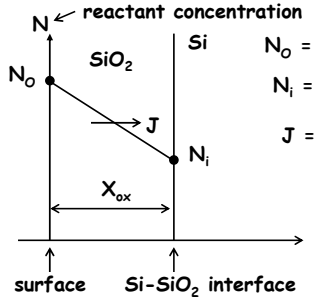
(2) As oxide builds up:



Reactant must diffuse to Si surface where the oxidation reaction takes place

↳ Growth rate governed more by rate of diffusion to the silicon-oxide interface

Oxidation Modeling (cont.)



N_O = reactant conc. at oxide surface [in cm^{-2}]

N_i = reactant conc. at Si-SiO_2 interface

J = reactant flux = $-D\frac{\partial N(x,t)}{\partial x}$ [Fick's 1st Law of Diffusion]

Diffusion coeff. [in μm/hr or m/s]

In the SiO_2:

$$J = D\frac{(N_O - N_i)}{X_{OX}} = \text{constant} \qquad (1)$$

[in # particles/(cm^2·s)]

Assumption that the reactant does not accumulate in the oxide.

Oxidation Modeling (cont.)

At the Si-SiO_2 interface:

Oxidation rate $\propto N_i$ $\therefore J \propto N_i \Rightarrow$ $\boxed{J = k_s N_i}$ (2)

Reaction rate constant @ Si-SiO_2 interface

Combining (1) and (2):

$$\left[N_i = \frac{J}{k_s}\right] \Rightarrow J = D\left(\frac{N_O - J/k_s}{X_{OX}}\right)$$

$$JX_{OX} = DN_O - \frac{DJ}{k_s} \rightarrow J\left(X_{OX} + \frac{D}{k_s}\right) = DN_O$$

$$\therefore \boxed{J = \frac{DN_O}{X_{OX} + \frac{D}{k_s}} = \text{Flux of reactants}}$$

Oxidation Modeling (cont.)

Find an expression for $X_{OX}(t)$:

oxidizing flux

Rate of change of oxide layer thickness w/time $\Big\} = \dfrac{dX_{OX}}{dt} = \dfrac{J}{M} = \dfrac{DN_O/M}{X_{OX} + D/k_s}$ (3)

# of molecules of oxidizing species incorporated into a unit volume of oxide $\Big\} = 2.2\times10^{22} cm^{-3}$ for O_2; $= 4.4\times10^{22} cm^{-3}$ for H_2O

Solve (3) for $X_{OX}(t)$: [Initial condition $X_{OX}(t=0) = X_i$]

$$\frac{dX_{OX}}{dt} = \frac{DN_O/M}{X_{OX} + D/k_s} \Rightarrow \int_{X_i}^{X_{OX}} \left(X_{OX} + \frac{D}{k_s}\right) dX_{OX} = \int_0^t \frac{DN_O}{M}\, dt$$

Oxide Thickness Versus Time

Result:

additional time required to go from $X_i \rightarrow X_{OX}$

time required to grow X_i [X_i = initial oxide thickness]

$$X_{OX}(t) = \frac{A}{2}\left\{\left[1 + \frac{4B}{A^2}(t+\tau)\right]^{1/2} - 1\right\}$$

where $A = \dfrac{2D}{k_s}$ $\qquad \tau = \dfrac{X_i^2}{B} + \dfrac{X_i}{(B/A)}$

$B = \dfrac{2DN_O}{M}$ $\qquad D = D_O \exp\left(-\dfrac{E_A}{kT}\right)$

[i.e., D governed by an Arrhenius relationship → temperature dependent]

Oxidation Modeling (cont.)

For shorter times:

$$\left[(t+\tau) << \frac{A^2}{4B}\right] \Rightarrow X_{OX}(t) = \underbrace{\left(\frac{B}{A}\right)}(t+\tau) \Rightarrow$$

oxide growth limited by reaction at the Si-SiO_2 interface

Taylor expansion (first term after 1's cancel)

linear growth rate constant

For long oxidation times: oxide growth diffusion-limited

$$\left[(t+\tau) >> \frac{A^2}{4B}\right] \Rightarrow X_{OX}(t) = \sqrt{B(t+\tau)} \approx \sqrt{Bt}$$

$t >> \tau$

Parabolic rate constant

Oxidation Rate Constants

Table 6–2 Rate constants describing (111) silicon oxidation kinetics at 1 Atm total pressure. For the corresponding values for (100) silicon, all C_2 values should be divided by 1.68.

Ambient	B	B/A
Dry O_2	$C_1 = 7.72 \times 10^2\ \mu m^2\ hr^{-1}$	$C_2 = 6.23 \times 10^6\ \mu m\ hr^{-1}$
	$E_1 = 1.23$ eV	$E_2 = 2.0$ eV
Wet O_2	$C_1 = 2.14 \times 10^2\ \mu m^2\ hr^{-1}$	$C_2 = 8.95 \times 10^7\ \mu m\ hr^{-1}$
	$E_1 = 0.71$ eV	$E_2 = 2.05$ eV
H_2O	$C_1 = 3.86 \times 10^2\ \mu m^2\ hr^{-1}$	$C_2 = 1.63 \times 10^8\ \mu m\ hr^{-1}$
	$E_1 = 0.78$ eV	$E_2 = 2.05$ eV

- Above theory is great … but usually, the equations are not used in practice, since measured data is available
  - Rather, oxidation growth charts are used

Oxidation Growth Charts

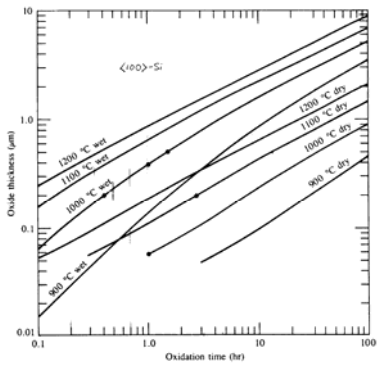


Fig. 3.1

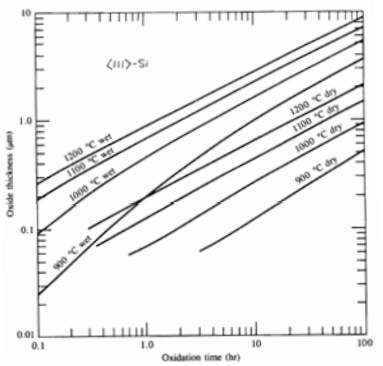
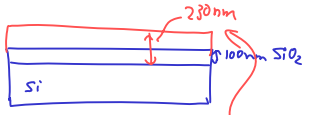


Fig. 3.2

Using the Oxidation Growth Charts

Example:

- <100> silicon
- Starting oxide thickness: X_i=100nm
- Want to do wet oxidation @ 1000°C to achieve X_{ox}=230nm
- What is the time *t* required for this?



Growth Chart for <100> Silicon

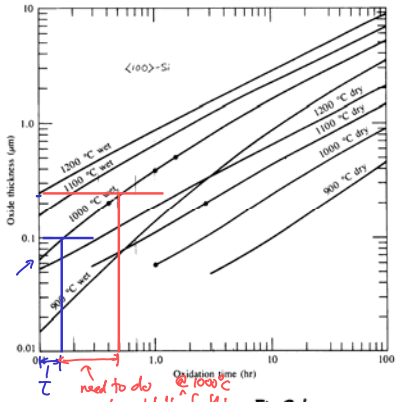


Fig. 3.1

Factors Affecting Oxidation

- In summary, oxide thickness is dependent upon:
  1. Time of oxidation
  2. Temperature of oxidation
  3. Partial pressure of oxidizing species ($\propto N_o$)
- Also dependent on:
  4. Reactant type:
     Dry O_2
     Water vapor ⇨ faster oxidation, since water has a higher solubility (i.e., D) in SiO_2 than O_2
  5. Crystal orientation:
     <111> ← faster, because there are more bonds available at the Si-surface
     <100> ← fewer interface traps; smaller # of unsatisfied Si-bonds at the Si-SiO_2 interface

Factors Affecting Oxidation

6. Impurity doping:
   P: increases linear rate const.
   no affect on parabolic rate constant
   faster initial growth → surface reaction rate limited
   B: no effect on linear rate const.
   increases parabolic rate const.
   faster growth over an initial oxide → diffusion faster

Thin Film Deposition

Thin Film Deposition

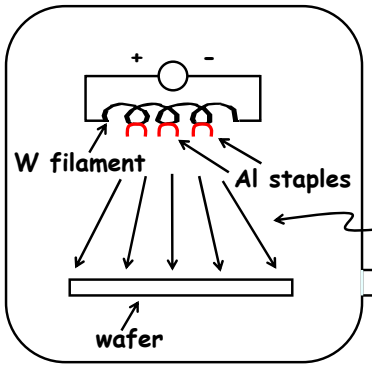
- Methods for film deposition:
  - Evaporation
  - Sputter deposition
  - Chemical vapor deposition (CVD)
  - Plasma enhanced chemical vapor deposition (PECVD)
  - Epitaxy
  - Electroplating
  - Atomic layer deposition (ALD)

Evaporation:

- Heat a metal (Al, Au) to the point of vaporization
- Evaporate to form a thin film covering the surface of the Si wafer
- Done under vacuum for better control of film composition

Evaporation

Filament Evaporation System:



1. Pump down to vacuum → reduces film contamination and allows better thickness control
2. Heat W filament → melt Al, wet filament
3. Raise temperature → evaporate Al

$$\text{mean free path} = \lambda = \frac{kT}{\sqrt{2}\pi Pd^2}$$

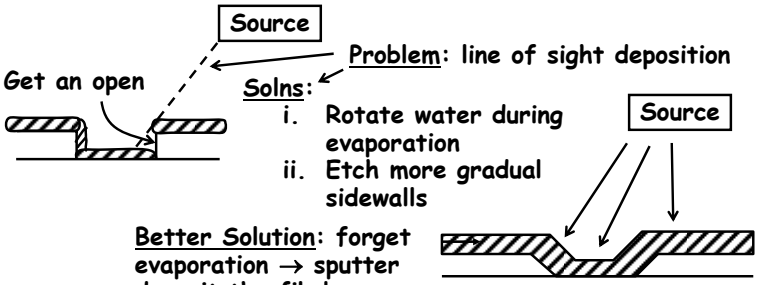
Vacuum Pump

k = Boltzmann Constant
T = temperature
P = pressure
d = diameter of gas molecule

Evaporation (cont.)

- λ can be ~60m for a 4Å particle at 10^{-4} Pa (~0.75 μTorr)
  - thus, at 0.75 μTorr, get straight line path from Al staple filament to wafer

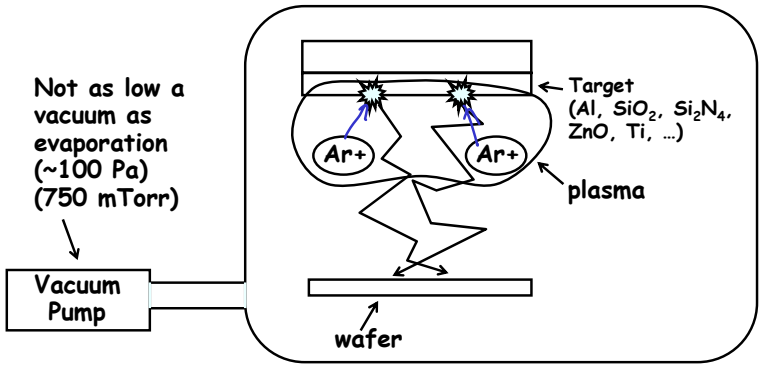
Problem: Shadowing & Step Coverage



Better Solution: forget evaporation → sputter deposit the film!

Sputter Deposition

- Use an energetic plasma to dislodge atoms from a material target, allowing the atoms to settle on the wafer surface



Sputter Deposition Process

- Step-by-step procedure:
  1. Pump down to vacuum

$$(\sim 100\ \text{Pa}) \rightarrow 1\ \text{Pa} = 9.8\times10^{-6}\ \text{atm}\left(\frac{760\ \text{Torr}}{\text{atm}}\right) = 0.0075012\ \text{Torr}$$

(1 Pa = 750 mTorr)

  2. Flow gas (e.g., Ar)
  3. Fire up plasma (create Ar+ ions) → apply dc-bias (or RF for non-conductive targets)
  4. Ar+ ions bombard target (dislodge atoms)
  5. Atoms make their way to the wafer in a more random fashion, since at this higher pressure, λ ~60μm for a 4Å particle; plus, the target is much bigger

- Result: better step coverage!

Problems With Sputtering

1. Get some Ar in the film
2. Substrate can heat up
   - up to ~350°C, causing nonuniformity across the wafer
   - but it still is more uniform than evaporation!
3. Stress can be controlled by changing parameters (e.g., flow rate, plasma power) from pass to pass, but repeatability is an issue

- Solution: use Chemical Vapor Deposition (CVD)

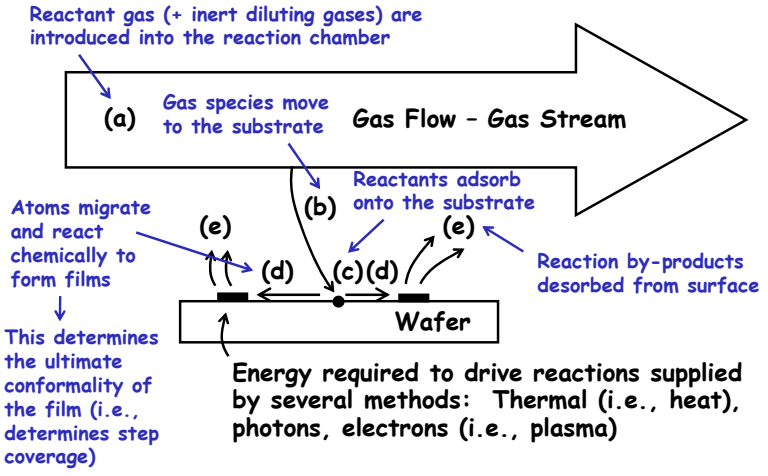
Chemical Vapor Deposition (CVD)

- Even better conformity than sputtering
- Form thin films on the surface of the substrate by thermal decomposition and/or reaction of gaseous compounds
  - Desired material is deposited directly from the gas phase onto the surface of the substrate
  - Can be performed at pressures for which λ (i.e., the mean free path) for gas molecules is small
  - This, combined with relatively high temperature leads to

Excellent Conformal Step Coverage!

  - Types of films: polysilicon, SiO_2, silicon nitride, SiGe, Tungsten (W), Molybdenum (M), Tantalum (Ta), Titanium (Ti), …

The CVD Process



The CVD Process (cont.)

Step-by-Step CVD Sequence:

Gas phase processes:
a) Reactant gases (+ inert diluting gases) are introduced into reaction chamber
b) Gas species move to the substrate

Surface processes:
c) Reactants adsorbed onto the substrate
d) Atoms migrate and react chemically to form films
This determines to a large extent whether or not a film is conformal (i.e. better step coverage)

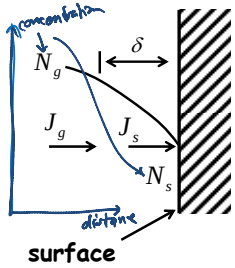
Not Conformal
low T
not enough adatom migration

Conformal
High T
Plenty of adatom migration

e) Reaction by-products desorbed and removed from reaction chamber

CVD Modeling

Simplified Schematic:



N_g = conc. of reactant molecules in the gas stream
N_s = conc. of reactant molecules at the surface
J_s = flux of gas molecules at the surface
J_g = flux of molecules diffusing in from the gas stream

Governing Equations:

$$J_s = k_s N_s \quad [k_s = \text{surface reaction rate const.}]$$

$$J_g = \left(\frac{\overline{D}_g}{\delta}\right)(N_g - N_s) = h_g(N_g - N_s)$$

Effective diffusion const. for the gas molecule

Vapor phase mass-transfer coefficient

CVD Modeling (cont.)

$$\underbrace{[J_s = J_g = J]}, \left[N_s = \frac{J_s}{k_s}\right] \rightarrow J = h_g\left(N_g - \frac{J}{k_s}\right) = h_g N_g - \frac{h_g J}{k_s}$$

Otherwise reactants will build up somewhere!

$$J\left(1 + \frac{h_g}{k_s}\right) = h_g N_g \rightarrow \boxed{J = \frac{k_s h_g}{k_s + h_g} N_g = (k_s || h_g) N_g}$$

$$\text{growth rate} = \frac{\text{flux}}{\#\,\text{molecules incorporated/unit volume}} = \frac{J}{N}$$

$$= \frac{J}{N} = \boxed{\frac{k_s h_g}{k_s + h_g}\frac{N_g}{N} = (k_s \,||\, h_g)\frac{N_g}{N} = \text{growth rate}}$$

CVD Modeling (cont.)

- Case: $k_s >> h_g$
  - surface reaction rate >> mass transfer rate

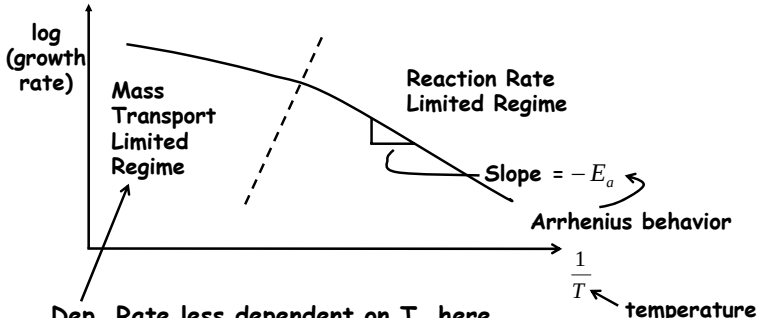
$$\text{growth rate} = h_g \frac{N_g}{N}$$ (mass-transfer-limited)

- Case: $h_g >> k_s$
  - mass transfer rate >> surface reaction rate

$$\text{growth rate} = k_s \frac{N_g}{N}$$ (surface-reaction-limited)

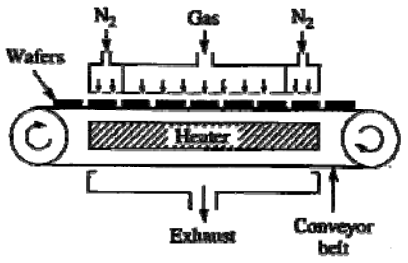
$$\sim R_o^{-E_a/kT}$$ (Arrhenius character)

Temperature Dependence of CVD



Dep. Rate less dependent on T, here
- for better control, better to operate here (@ higher T)

Atmospheric Pressure Reactor (APCVD)



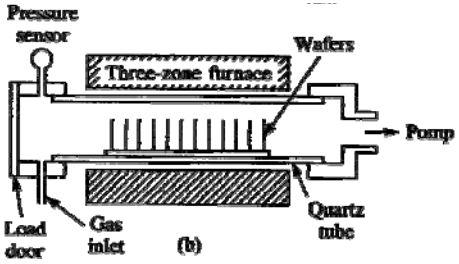
- Once used for silicon dioxide passivation in integrated circuits
- Substrates fed continuously
- Large diameter wafers
- Need high gas flow rates
- Mass transport-limited regime (high pressure, so tougher for gas to get to the wafer surface)

- Problems/Issues:
  - Wafers lay flat, and thus, incorporate foreign particles
  - Poor step coverage

Low Pressure Reactor (LPCVD)

- Many films available: polysilicon, SiGe, Si_3N_4, SiO_2, phosphosilicate glass (PSG), BPSG, W

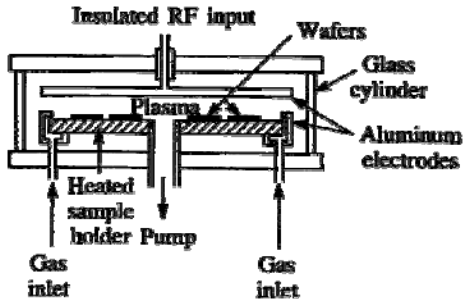
- Temp.: 300 → 1150°C
- Press.: 30 → 250 Pa (200mTorr → 2Torr)
- Reaction rate limited; reduced pressure gives gas molecular high diffusivity; can supply reactants very fast!
- Can handle several hundred wafers at a time
- Excellent uniformity

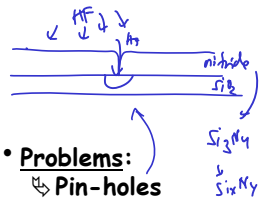


- Problems:
  - Low dep. rate (compared to atm.)
  - Higher T (than atmospheric)
  - In hot wall reactors, get deposition on tube walls (must clean)

Plasma-Enhanced CVD Reactor (PECVD)

- RF-induced glow discharge + thermal energy to drive reactions → allows lower temperature deposition with decent conformability
- Still low pressure





- Problems:
  - Pin-holes
  - Non-stoichiometric films
  - Incorporation of H_2, N_2, O_2 contaminants in film; can lead to outgassing or bubbling in later steps

Polysilicon CVD

Polysilicon Deposition:

$$SiH_4 \xrightarrow{600^\circ C} Si + 2H_2$$ (thermal decomposition of silane)

→ Fairly high temperature → conformal

(conformal → high T)

LPCVD (25 to 150 Pa) → 100-200Å/min

- In situ doping of polysilicon:
  - n-type: add PH_3 (phosphine) or Arsine gases (but greatly reduces dep. rate)
  - p-type: add diborane gas (greatly increases dep. Rate)

Silicon Oxide CVD

Silicon Dioxide Deposition:

- After metallization (e.g., over aluminum)
  - Temperature cannot exceed the Si-Al eutectic pt.: 577°C
  - Actually, need lower than this (<500°C) to prevent hillocks from growing on Al surfaces
  - Similar issues for copper (Cu) metallization
- Low temperature reactions:

LPCVD LTO Reactions:

$$SiH_4 + O_2 \xrightarrow[300\text{-}500^\circ C]{} SiO_2 + 2H_2$$ (silane)

$$4PH_3 + 5O_2 \xrightarrow[300\text{-}500^\circ C]{} 2P_2O_5 + 6H_2$$ (phosphine)

P_2O_5: Phosphosilicate glass (PSG)

- Above reactions: not very conformal step coverage → need higher T for this

Silicon Oxide CVD (cont.)

- Phosphosilicate glass can be reflown
  - 6-8 wt. % allows reflow @ 1000-1100°C
  - Very useful to achieve smoother topography
  - Lower concentration → won't reflow
  - Higher concentration → corrodes Al if moisture is present
  - 5-15% P can be used as a diffusion source to dope Si

- Before metallization:
  - Can use higher temperature → better uniformity and step coverage

HTO:

$$SiCl_2H_2 + 2N_2O \xrightarrow[\sim 900^\circ C]{} SiO_2 + 2N_2 + 2HCl$$

(dichlorosilane) (Nitrous oxide) (nice conformal step coverage)

or …

Silicon Oxide CVD (cont.)

$Si(OC_2H_5)_4 \xrightarrow{650\text{-}750^\circ C} SiO_2 + \text{by-products}$

(Tetraethylorthosilicate) (TEOS)

(excellent uniformity & conformal step coverage)

Silicon Nitride CVD

Silicon Nitride Deposition:

- First, note that thermal growth is possible:
  - Si in NH_3 @ 1000-1100°C
  - But very slow growth rate, thus, impractical
- LPCVD reactions:

Silane reaction: $3SiH_4 + 4NH_3 \xrightarrow[\text{(Atm. Press.)}]{700\text{-}900^\circ C} Si_3N_4 + 12H_2$

Dichlorosilane reaction:

$3SiCl_2H_2 + 4NH_3 \xrightarrow[\text{(LPCVD)}]{700\text{-}800^\circ C} Si_3N_4 + 6HCl + 6H_2$

Increase and T = 835°C ⟶ Si rich nitride ⟶ low stress

Problem: Clobbers your pumps! Expensive to maintain!

Silicon Nitride CVD (cont.)

- Comments on LPCVD nitride films:
  - Hydrogen rich: ~8% H_2
  - High internal tensile stresses: films >1000Å crack and peel due to excessive stress
  - Can get 2μm films with Si-rich nitride
  - LPCVD gives high resistivity (10^{16} Ω-cm) and dielectric strength (10 MV/cm)

PECVD Nitride:

$SiH_4 + N_2 \xrightarrow{\text{Nitrogen discharge}} 2SiNH + 3H_2$

or

$SiH_4 + NH_3 \xrightarrow[\text{Ar plasma}]{} SiNH + 3H_3$

PECVD films:
- Non-stoichiometric nitride
- 20-25% H_2 content
- Can control stress
- $(10^6 \Omega - cm)$ resistivity

Metal CVD

CVD Metal Deposition:

Tungsten (W) – deposited by thermal, plasma or optically-assisted decomposition

$WF_6 \longrightarrow W + 3F_2$

or via reaction with H_2:

$WF_6 + 3H_2 \longrightarrow W + 6HF$

Other Metals – Molybdenum (Mo), Tantalum (Ta), and Titanium (Ti)

$2MCl_5 + 5H_2 \longrightarrow 2M + 10HCl,$

where M = Mo, Ta, or Ti

(Even Al can be CVD'ed with tri-isobutyl Al … but other methods are better.)

(Cu is normally electroplated)