EE C245 – ME C218
Introduction to MEMS Design
Fall 2011

Prof. Clark T.-C. Nguyen

Dept. of Electrical Engineering & Computer Sciences
University of California at Berkeley
Berkeley, CA 94720

Lecture Module 3: Oxidation & Film Deposition

Lecture Outline

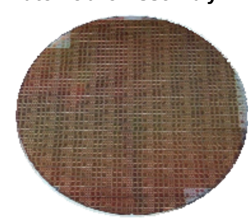
- Reading: Senturia, Chpt. 3; Jaeger, Chpt. 2, 3, 6
  - Example MEMS fabrication processes
  - Oxidation
  - Film Deposition
    - Evaporation
    - Sputter deposition
    - Chemical vapor deposition (CVD)
    - Plasma enhanced chemical vapor deposition (PECVD)
    - Epitaxy
    - Atomic layer deposition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

MEMS Fabrication

Making Mechanical Devices

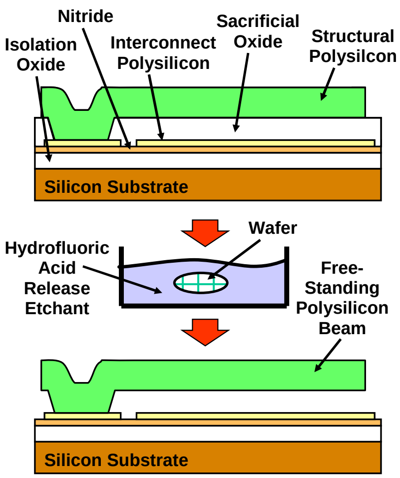
- How best does one make a mechanical product?
- Assembly line production?
  - Pick and place parts
  - Used for many macroscopic mechanical products
  - Robotic automation greatly reduces cost
- *Problem*: difficult to do this with MEMS-scale parts (but not impossible, as we'll soon see …)
- *Solution*: 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

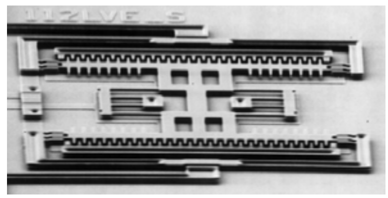


CMOS Integrated Circuit Wafer

Polysilicon Surface-Micromachining

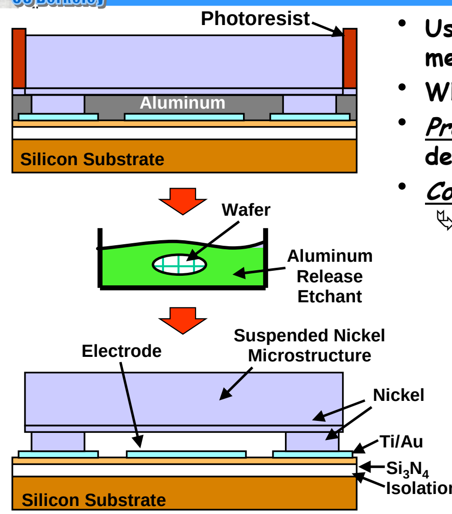


- Uses IC fabrication instrumentation exclusively
- *Variations*: sacrificial layer thickness, fine- vs. large-grained polysilicon, *in situ* vs. $POCL_3$-doping

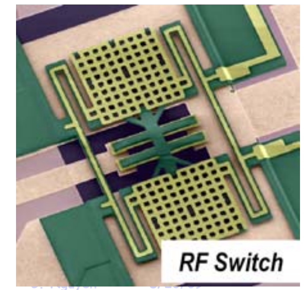


300 kHz Folded-Beam Micromechanical Resonator

Electroplating: Metal MEMS



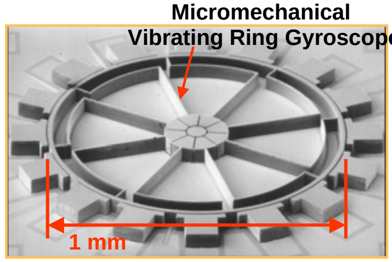
- Use electroplating to obtain metal μstructures
- When thick: call it "LIGA"
- *Pros*: fast low temp deposition, very conductive
- *Cons*: drift, low mech. *Q*
  - but may be solvable?



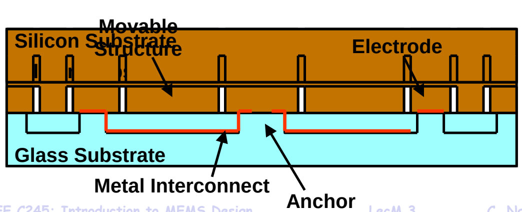
Bulk Micromachining and Bonding

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

Micromechanical Vibrating Ring Gyroscope



[Najafi, Michigan]



[Pisano, UC Berkeley]

Microrotor (for a microengine)

Oxidation

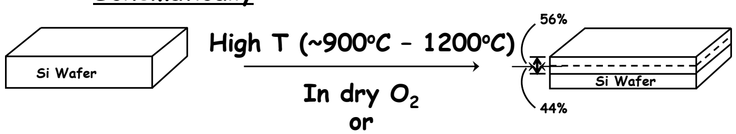
Thermal Oxidation of Silicon

- 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: $Si + O_2 \rightarrow SiO_2$

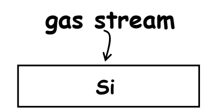
For water vapor: $Si + 2H_2O \rightarrow SiO_2 + 2H_2$

Schematically:



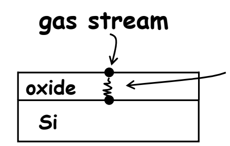
Oxidation Modeling

(1) Initially: (no oxide @ surface)



↳ Growth rate determined by reaction rate @ the surface

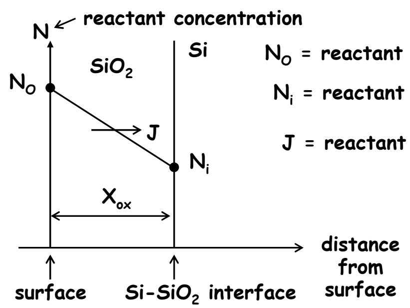
(2) As oxide builds up:



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

Diffusion coeff. [in μm/hr or m/s]

In the SiO$_2$: $\boxed{J = D\dfrac{(N_O - N_i)}{X_{OX}}}$ = constant (1)

[in # particles/(cm²•s)]

Assumption that the reactant does not accumulate in the oxide.

Oxidation Modeling (cont.)

At the Si-SiO$_2$ interface:

Oxidation rate $\propto N_i$ ∴ $J \propto N_i$ $\Longrightarrow$ $\boxed{J = k_s N_i}$ (2)

Reaction rate constant @ Si-SiO$_2$ interface

Combining (1) and (2):

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

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

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

Oxidation Modeling (cont.)

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

oxidizing flux

$$\left.\begin{array}{l}\text{Rate of change of oxide}\\\text{layer thickness w/time}\end{array}\right\} = \frac{dX_{OX}}{dt} = \frac{J}{M} = \frac{DN_O/M}{X_{OX} + D/k_s} \quad \text{(3)}$$

$$\left.\begin{array}{l}\text{\# of molecules of oxidizing}\\\text{species incorporated into a}\\\text{unit volume of oxide}\end{array}\right\} \begin{array}{l} = 2.2\times10^{22}cm^{-3} \text{ for } O_2 \\ = 4.4\times10^{22}cm^{-3} \text{ for } H_2O\end{array}$$

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

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

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

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

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

[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

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

$t >> \tau$

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	$C_1 = 7.72 \times 10^2\ \mu m^2\ hr^{-1}$ (D_o)	$C_2 = 6.23 \times 10^6\ \mu m\ hr^{-1}$
	$E_1 = 1.23$ eV (E_A)	$E_2 = 2.0$ 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

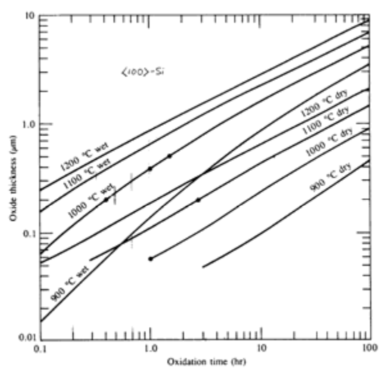


Fig. 3.1

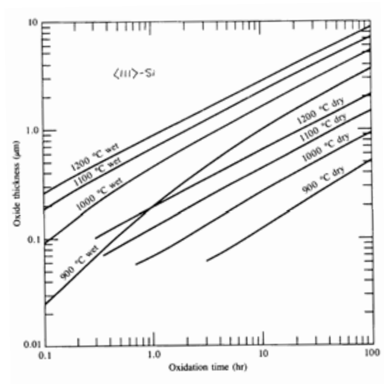


Fig. 3.2

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

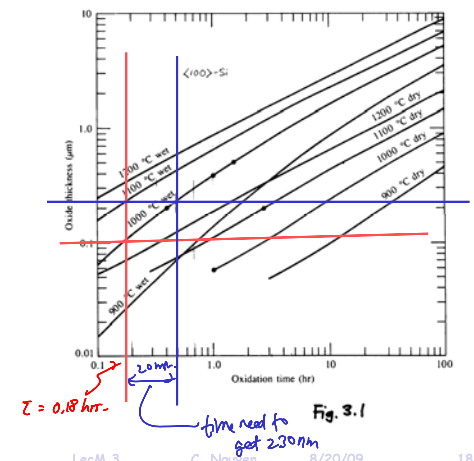


Fig. 3.1

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

UC Berkeley

Thin Film Deposition

UC Berkeley

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)

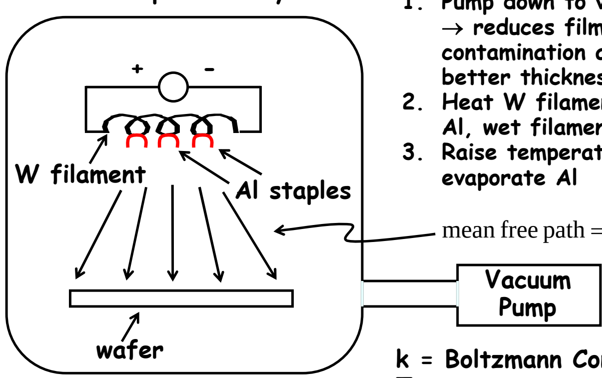
Evaporation:

- 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

UC Berkeley

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

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

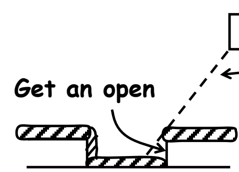
k = Boltzmann Constant
T = temperature
P = pressure
d = diameter of gas molecule

UC Berkeley

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

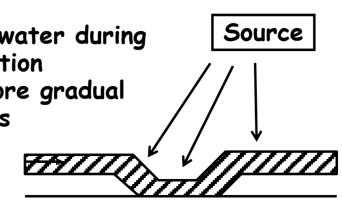
Problem: Shadowing & Step Coverage



Get an open

Problem: line of sight deposition

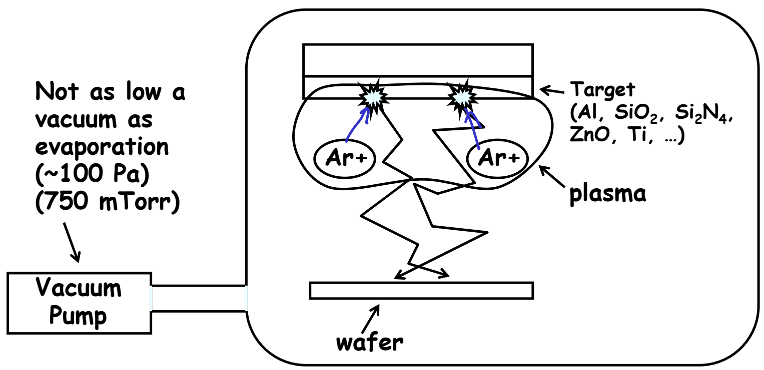
Solns:
i. Rotate water during evaporation
ii. Etch more gradual sidewalls



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

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

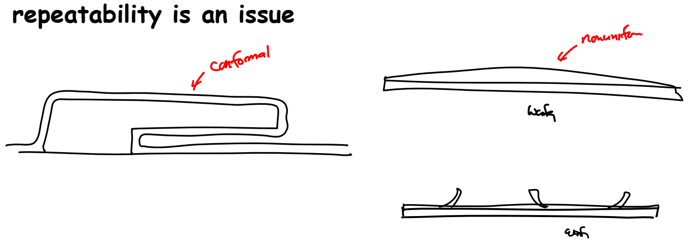
7.5 mTorr

  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)

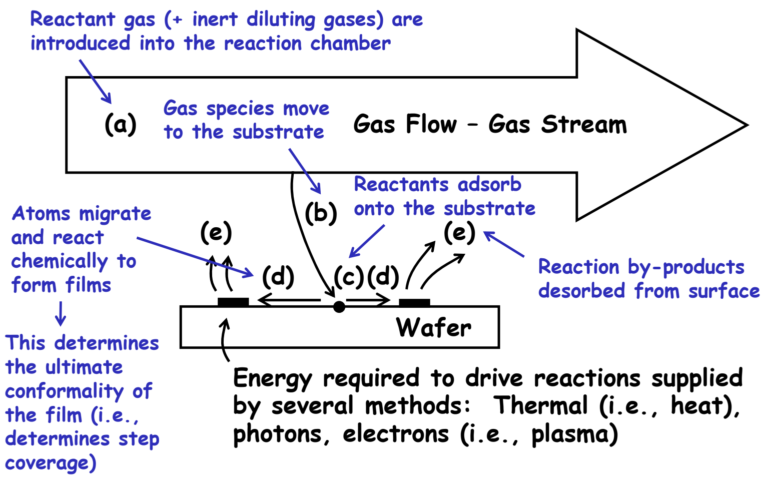
Chemical Vapor Deposition (CVD)

- 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

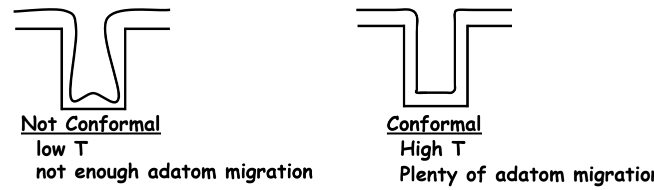


The CVD Process (cont.)

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

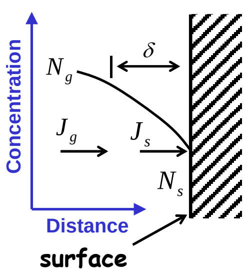
Surface processes
- c) Reactants adsorbed onto the substrate
- d) Atoms migrate and react chemically to form films
  This determines to a large extent whether or not a film is conformal (i.e. better step coverage)



- 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:

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

Effective diffusion const. for the gas molecule

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

Vapor phase mass-transfer coefficient

CVD Modeling (cont.)

$$\underbrace{[J_s = J_g = J]}_{}, \left[N_s = \frac{J_s}{k_s}\right]$$

Otherwise reactants will build up somewhere!

$$J = h_g\left(N_g - \frac{J}{k_s}\right) = h_g N_g - \frac{h_g J}{k_s}$$

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

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

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

CVD Modeling (cont.)

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

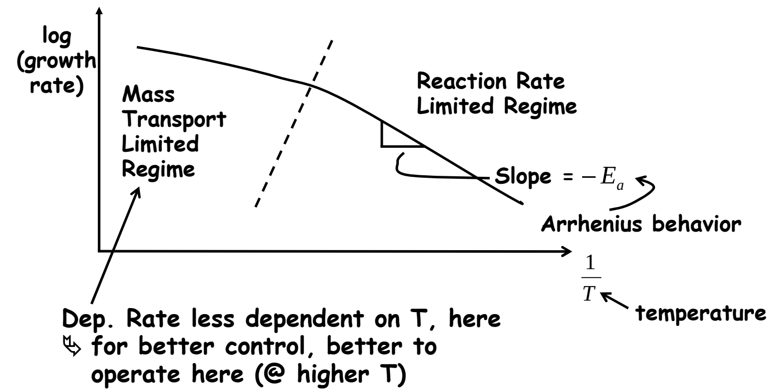
$$\boxed{\text{growth rate} = h_g \frac{N_g}{N}}$$ (mass-transfer-limited)

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

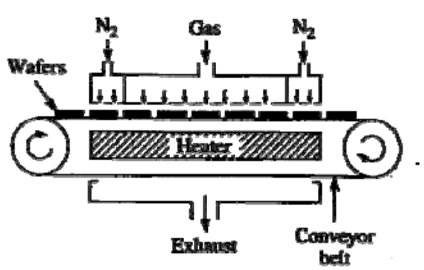
$$\boxed{\text{growth rate} = k_s \frac{N_g}{N}}$$ (surface-reaction-limited)

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

Temperature Dependence of CVD



Atmospheric Pressure Reactor (APCVD)



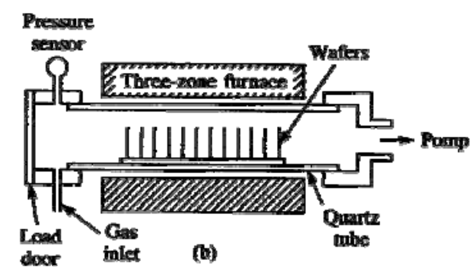
- Once used for silicon dioxide passivation in integrated circuits
- Substrates fed continuously
- Large diameter wafers
- Need high gas flow rates
- Mass transport-limited regime (high pressure, so tougher for gas to get to the wafer surface)

- 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

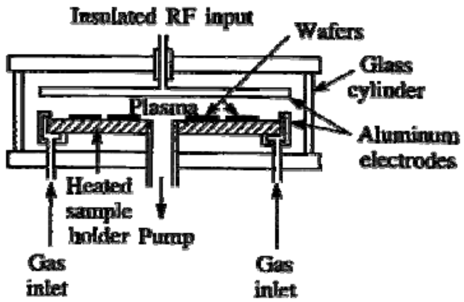
- Temp.: 300 → 1150°C
- Press.: 30 → 250 Pa (200mTorr → 2Torr)
- Reaction rate limited; reduced pressure gives gas molecular high diffusivity; can supply reactants very fast!
- Can handle several hundred wafers at a time
- Excellent uniformity



- 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:

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

600°C → 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:

$$SiH_4 + O_2 \xrightarrow{300\text{-}500°C} SiO_2 + 2H_2$$
(silane)

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

$2P_2O_5$ ← Phosphosilicate glass (PSG)

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