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EE C245 – ME C218
Introduction to MEMS Design
Fall 2012

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Lecture Module 3: Oxidation & Film Deposition

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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

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MEMS Fabrication

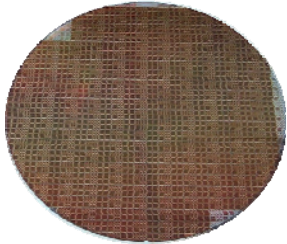EE C245: Introduction to MEMS Design   LecM 3   C. Nguyen   8/20/09   3

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
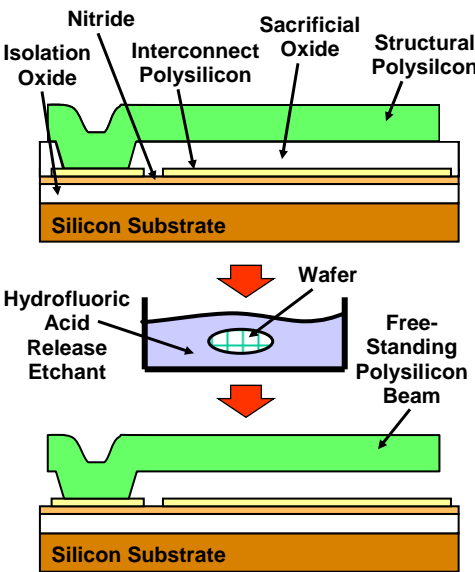
Automobile Assembly Line
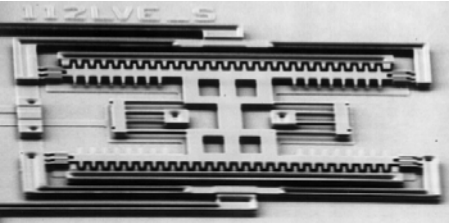
CMOS Integrated Circuit Wafer

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Polysilicon Surface-Micromachining

Nitride
Sacrificial Oxide
Structural Polysilcon
Isolation Oxide
Interconnect Polysilicon

Silicon Substrate

Hydrofluoric Acid Release Etchant
Wafer
Free-Standing Polysilicon Beam

Silicon Substrate

- 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
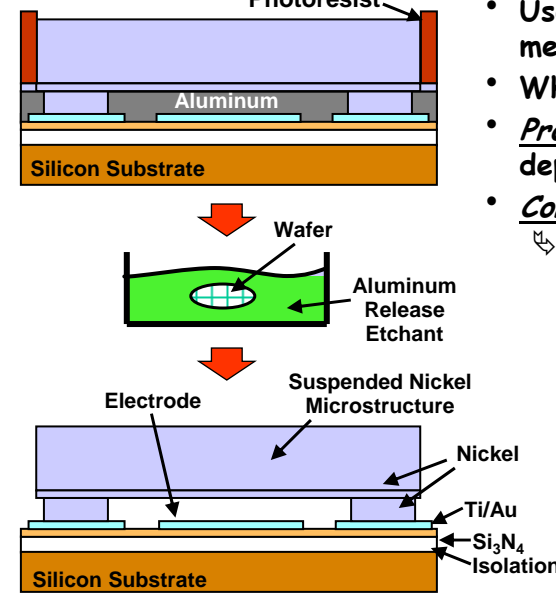
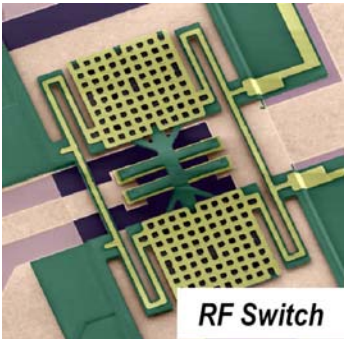EE C245: Introduction to MEMS Design   LecM 3   C. Nguyen   8/20/09   5

Electroplating: Metal MEMS

Photoresist

Aluminum

Silicon Substrate

Wafer
Aluminum Release Etchant

Electrode
Suspended Nickel Microstructure
Nickel
Ti/Au
Si$_3$N$_4$ Isolation

Silicon Substrate

- 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?

RF Switch
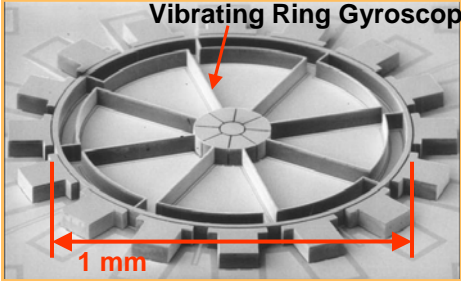
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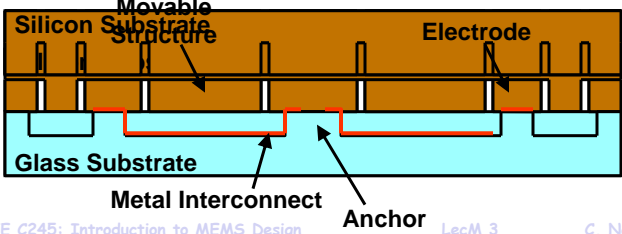
Bulk Micromachining and Bonding

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- 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

1 mm

[Najafi, Michigan]

[Pisano, UC Berkeley]

Silicon Substrate
Movable Structure
Electrode

Glass Substrate

Metal Interconnect
Anchor

Microrotor (for a microengine)

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Oxidation

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Thermal Oxidation of Silicon

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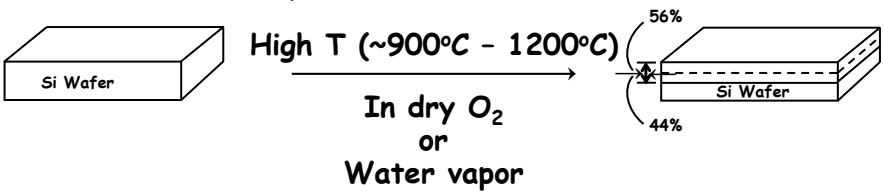- Enabling reactions:

For dry oxygen:

$Si + O_2 \rightarrow SiO_2$

For water vapor:

$Si + 2H_2O \rightarrow SiO_2 + 2H_2$

Schematically:
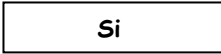
Si Wafer

High T (~900°C – 1200°C)

In dry O_2
or
Water vapor

56%

Si Wafer

44%
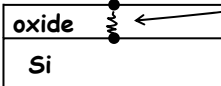
Oxidation Modeling

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(1) <u>Initially</u>: (no oxide @ surface)

gas stream

Si

↳ Growth rate determined by reaction rate @ the surface

(2) <u>As oxide builds up</u>:

gas stream

oxide

Si

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

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Oxidation Modeling (cont.)

N ← reactant concentration

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$_2$: $J = D\dfrac{(N_O - N_i)}{X_{OX}}$ = **constant**   (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 $\propto N_i$ $\Longrightarrow$ $J = k_s N_i$ (2)

Reaction rate constant @ Si-SiO$_2$ interface

Combining (1) and (2):

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

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

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

Oxidation Modeling (cont.)

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

oxidizing flux

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

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

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

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

Oxide Thickness Versus Time

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

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

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

Oxidation Modeling (cont.)

For shorter times:

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

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$_2$	$C_1 = 7.72 \times 10^2\ \mu m^2\ hr^{-1}$ $E_1 = 1.23\ eV$	$C_2 = 6.23 \times 10^6\ \mu m\ hr^{-1}$ $E_2 = 2.0\ eV$
Wet O$_2$	$C_1 = 2.14 \times 10^2\ \mu m^2\ hr^{-1}$ $E_1 = 0.71\ eV$	$C_2 = 8.95 \times 10^7\ \mu m\ hr^{-1}$ $E_2 = 2.05\ eV$
H$_2$O	$C_1 = 3.86 \times 10^2\ \mu m^2\ hr^{-1}$ $E_1 = 0.78\ eV$	$C_2 = 1.63 \times 10^8\ \mu m\ hr^{-1}$ $E_2 = 2.05\ eV$

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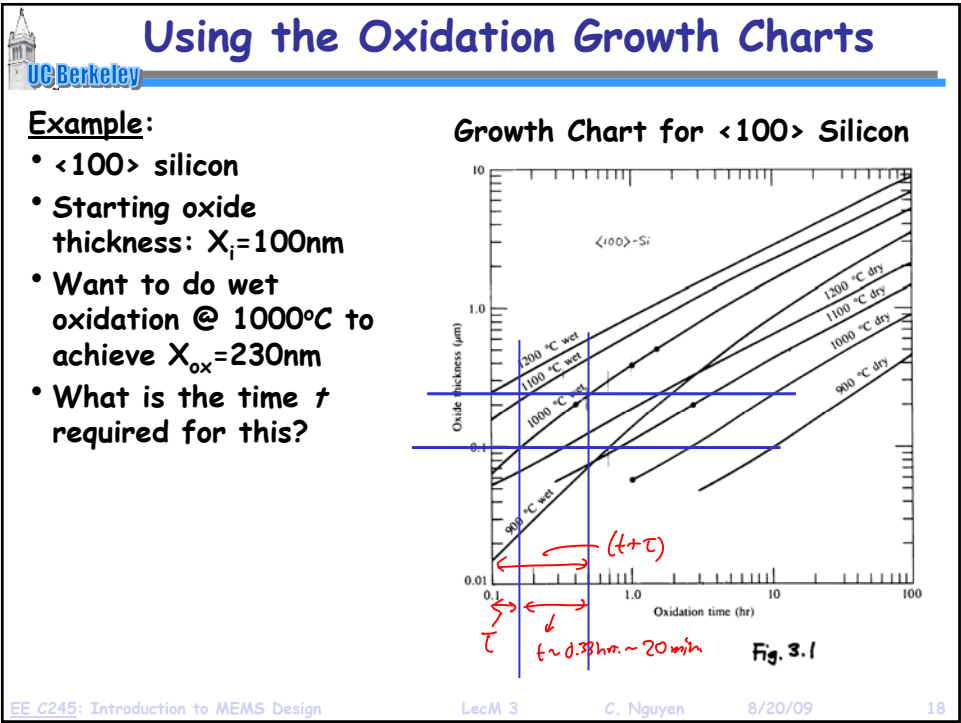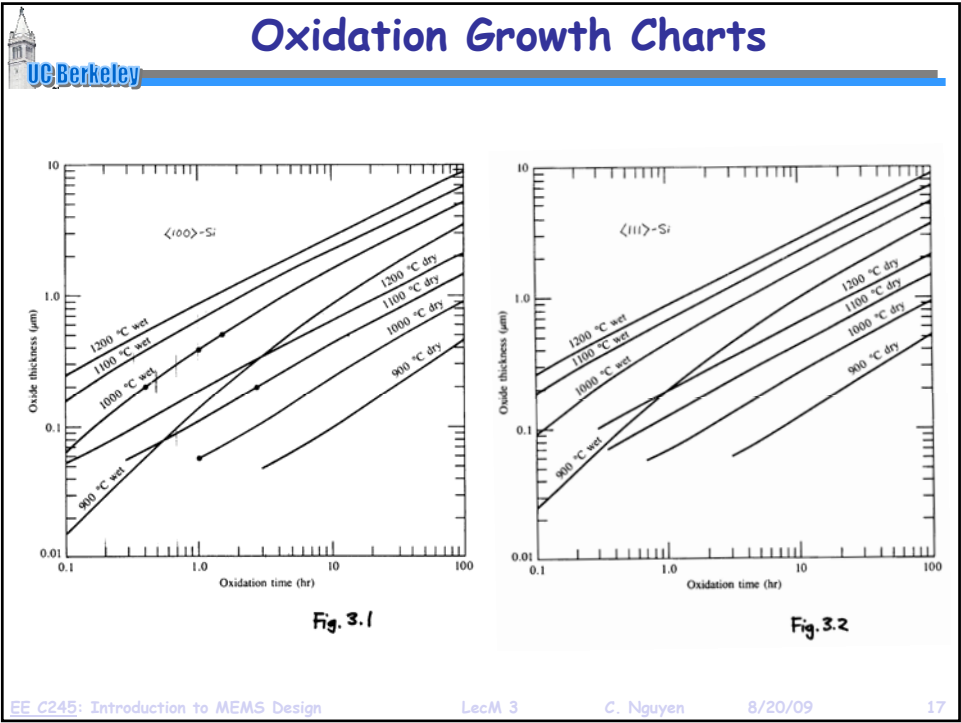 ⮎ **Rather, oxidation growth charts are used**

Oxidation Growth Charts

Fig. 3.1   Fig. 3.2

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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

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Factors Affecting Oxidation

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- 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 $\Rightarrow$ faster oxidation, since water has a
                higher solubility (i.e., D) in SiO_2 than O_2
    5. Crystal orientation:
        <111> $\leftarrow$ faster, because there are more bonds
                available at the Si-surface
        <100> $\leftarrow$ fewer interface traps; smaller # of
                unsatisfied Si-bonds at the Si-SiO_2 interface

Factors Affecting Oxidation

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6. Impurity doping:
    P: increases linear rate const.
        no affect on parabolic rate constant
        faster initial growth $\rightarrow$ surface reaction rate limited
    B: no effect on linear rate const.
        increases parabolic rate const.
        faster growth over an initial oxide $\rightarrow$ 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
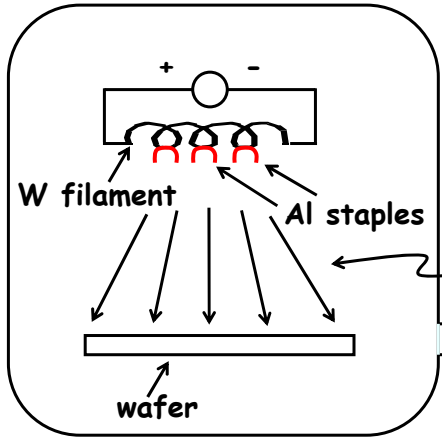 - Electroplating
  - Atomic layer deposition (ALD)

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

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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

W filament

Al staples

+ −

wafer

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

Vacuum Pump

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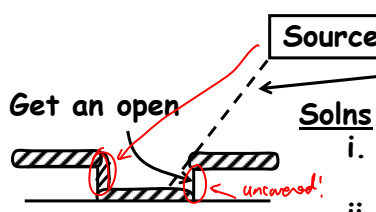T = temperature
P = pressure
d = diameter of gas molecule

Evaporation (cont.)

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- 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

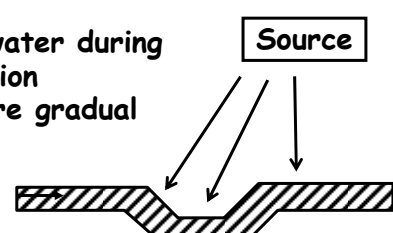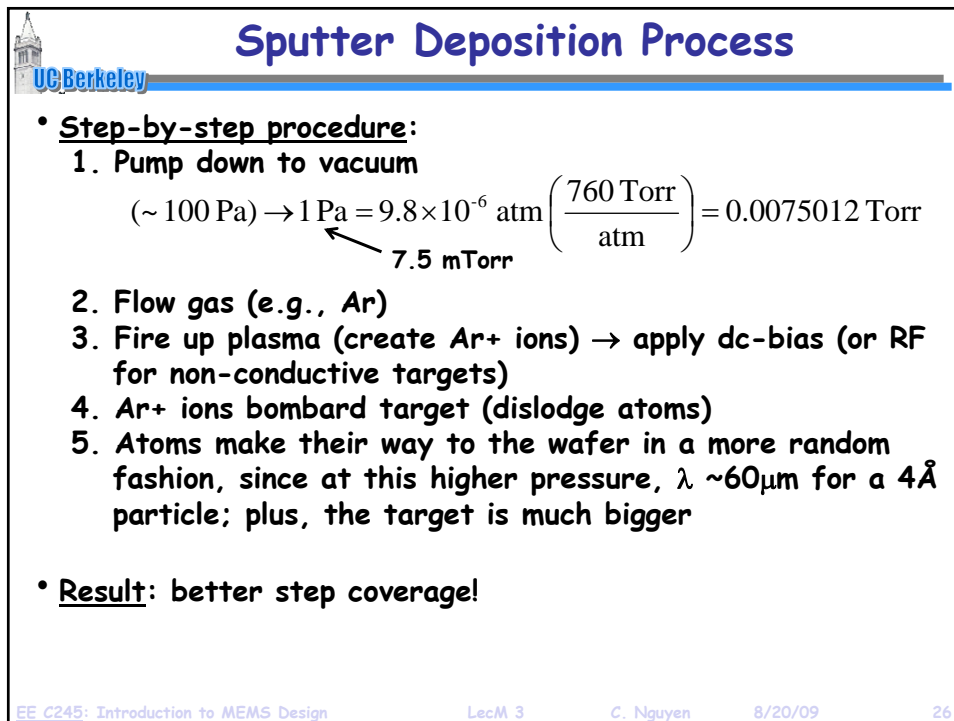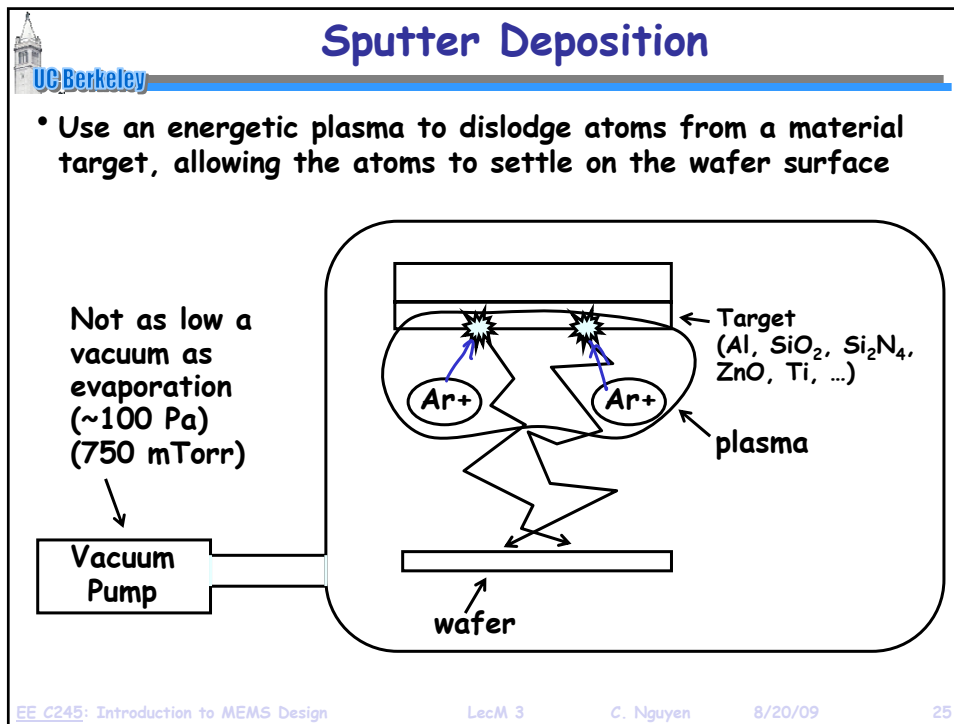**Problem**: Shadowing & Step Coverage

Source

Get an open

uncovered!

Problem: line of sight deposition

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

Better Solution: forget evaporation → sputter deposit the film!

Source

Sputter Deposition

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

Not as low a vacuum as evaporation (~100 Pa) (750 mTorr)

Vacuum Pump

Target (Al, SiO_2, Si_2N_4, ZnO, Ti, …)

Ar+   Ar+

plasma

wafer

Sputter Deposition Process

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

  $$(\sim 100\,\text{Pa}) \rightarrow 1\,\text{Pa} = 9.8 \times 10^{-6}\,\text{atm} \left(\frac{760\,\text{Torr}}{\text{atm}} \right) = 0.0075012\,\text{Torr}$$

  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), …

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The CVD Process

Reactant gas (+ inert diluting gases) are introduced into the reaction chamber

(a) Gas species move to the substrate   **Gas Flow – Gas Stream**

(b) Reactants adsorb onto the substrate

Atoms migrate and react chemically to form films

(e)   (d)   (c)(d)   (e)

Reaction by-products desorbed from surface

This determines the ultimate conformality of the film (i.e., determines step coverage)

Wafer

Energy required to drive reactions supplied by several methods: Thermal (i.e., heat), photons, electrons (i.e., plasma)

The CVD Process (cont.)

Step-by-Step CVD Sequence:

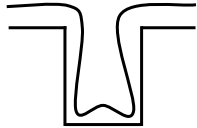Gas phase processes
- a) Reactant gases (+ inert diluting gases) are introduced into reaction chamber
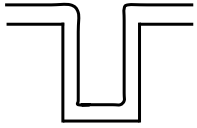- b) Gas species move to the substrate

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
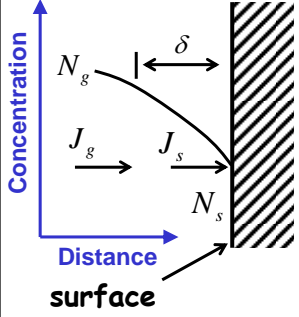
CVD Modeling

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

surface

Governing Equations:

Effective diffusion const. for the gas molecule

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

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

Vapor phase mass-transfer coefficient

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CVD Modeling (cont.)

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

Otherwise reactants will build up somewhere!

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

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

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

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

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CVD Modeling (cont.)

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

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

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

$$\boxed{\text{growth rate} = k_s \frac{N_g}{N}} \quad \text{(surface-reaction-limited)}$$
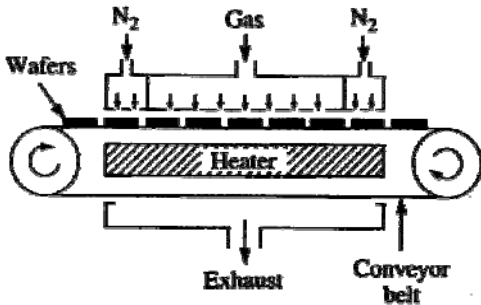
$$\sim R_o^{-E_a/kT} \text{ (Arrhenius character)}$$

Temperature Dependence of CVD

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log (growth rate)

Mass Transport Limited Regime

Reaction Rate Limited Regime

Slope = $-E_a$

Arrhenius behavior

$\frac{1}{T}$ ← temperature

Dep. Rate less dependent on T, here
⇨ for better control, better to operate here (@ higher T)
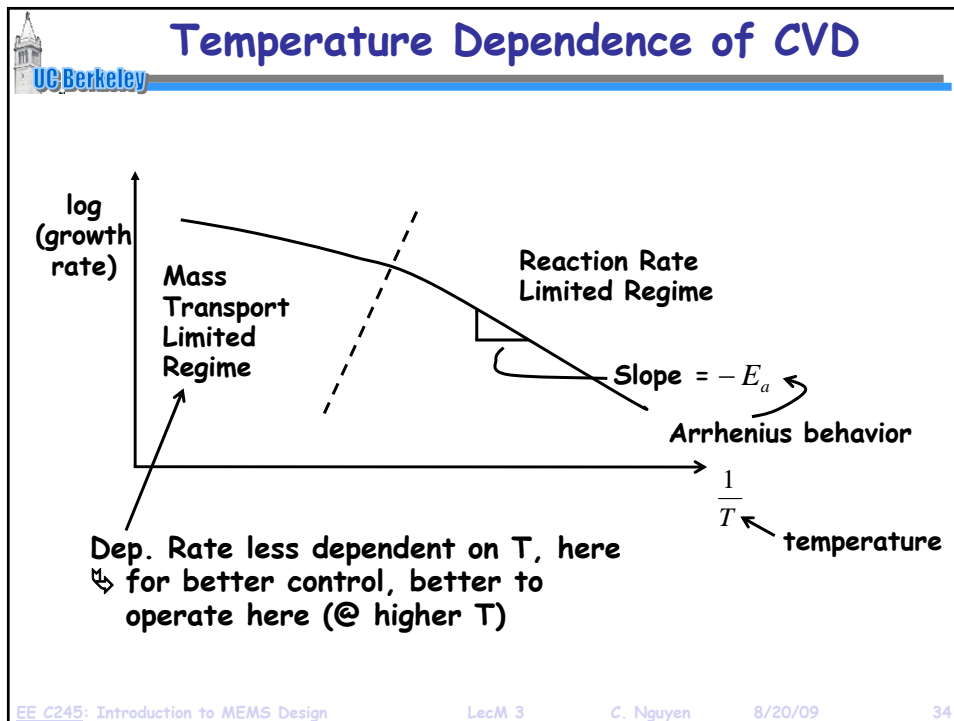
Atmospheric Pressure Reactor (APCVD)

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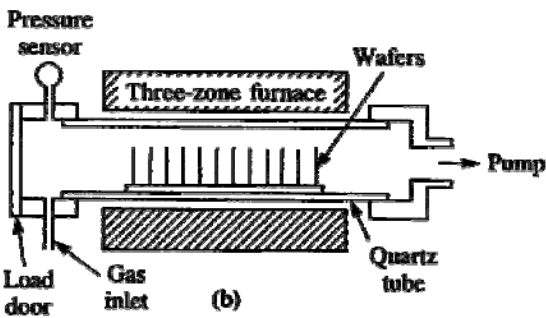
- Problems/Issues:
  ↳ Wafers lay flat, and thus, incorporate foreign particles
  ↳ Poor step coverage

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Low Pressure Reactor (LPCVD)

- Many films available: polysilicon, SiGe, Si_3N_4, SiO_2, phoshosilicate 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:
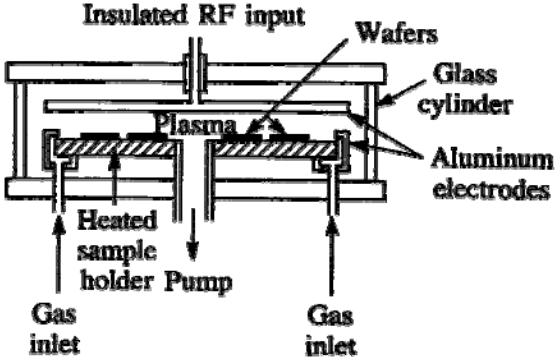 ↳ Low dep. rate (compared to atm.)
  ↳ Higher T (than atmospheric)
  ↳ In hot wall reactors, get deposition on tube walls (must clean)

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Plasma-Enhanced CVD Reactor (PECVD)

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- 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

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Polysilicon CVD

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Polysilicon Deposition:

→ Fairly high temperature → conformal

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

(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)

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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
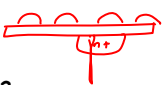 ↳ Similar issues for copper (Cu) metallization

• Low temperature reactions:

$$\text{LPCVD} \atop \text{LTO} \atop \text{Reactions} \begin{cases} \underset{\text{(silane)}}{SiH_4 + O_2} \xrightarrow{\text{300-500°C}} SiO_2 + 2H_2 \\ \underset{\text{(phosphine)}}{4PH_3 + 5O_2} \xrightarrow{\text{300-500°C}} 2P_2O_5 + 6H_2 \end{cases}$$

  Phosphosilicate glass (PSG)

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

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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

$$\text{HTO} \begin{cases} \underset{\text{(dichlorosilane)}}{SiCl_2H_2} + 2N_2O \xrightarrow{\text{~900°C}} SiO_2 + 2N_2 + 2HCl \\ \quad\quad\quad\quad \underset{\text{oxide)}}{\text{(Nitrous}} \quad\quad \underset{\text{step coverage)}}{\text{(nice conformal}} \end{cases}$$
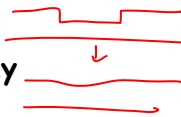
or ...

Silicon Oxide CVD (cont.)

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$$Si(OC_2H_5)_4 \longrightarrow SiO_2 + \text{by-products}$$

650-750°C

(Tetraethylorthosilicate)
(TEOS)

(excellent uniformity &
conformal step coverage)