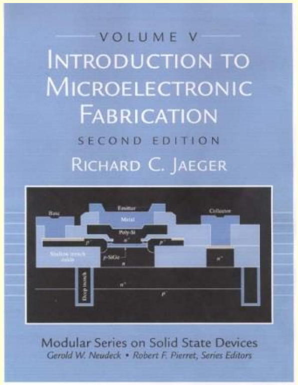
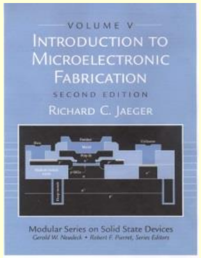
Introduction to Microelectronic Fabrication

Chapter 3

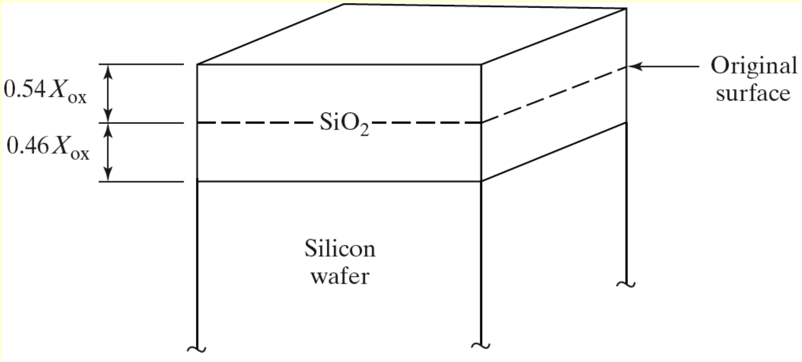
Thermal Oxidation of Silicon



Thermal Oxidation of Silicon



- Silicon Dioxide
  - High quality electrical insulator
  - Diffusion/implantation barrier
  - Passivates silicon surface



Dry Oxidation

$$Si + O_2 \rightarrow SiO_2$$

Wet Oxidation

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

Growth Occurs 54% above and 46% below original surface as silicon is consumed

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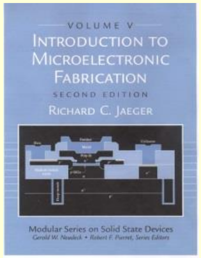
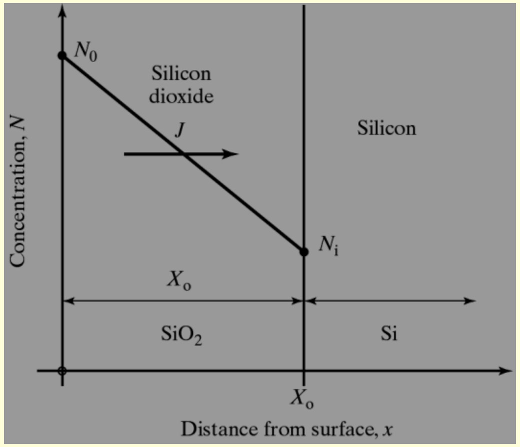
Thermal Oxidation
Fick's First Law of Diffusion



Particle flux J is proportional to the negative of the gradient of the particle concentration

$$J = -D\frac{\partial N}{\partial x} \qquad D = \text{diffusion coefficient}$$

Particles move from a region of high concentration to one of low concentration



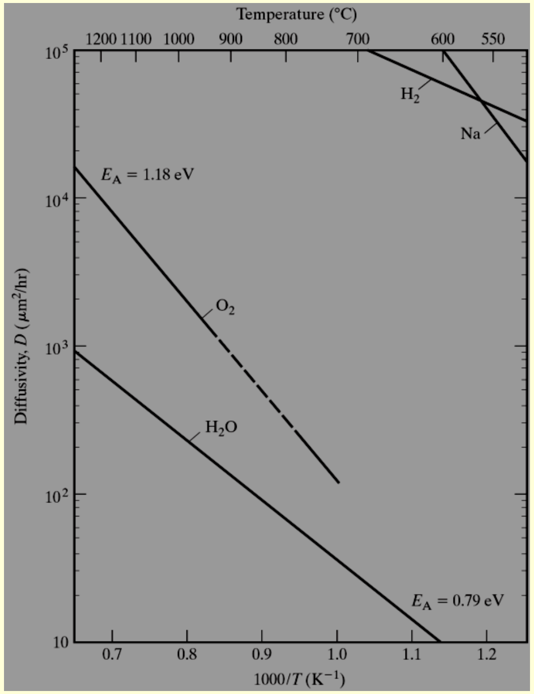


FIGURE 3.1

Diffusivities of hydrogen, oxygen, sodium, and water vapor in silicon glass. Copyright John Wiley & Sons, Inc. Reprinted with permission from Ref. [4].

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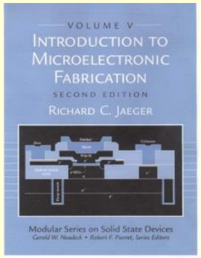
Thermal Oxidation
Fick's First Law of Diffusion



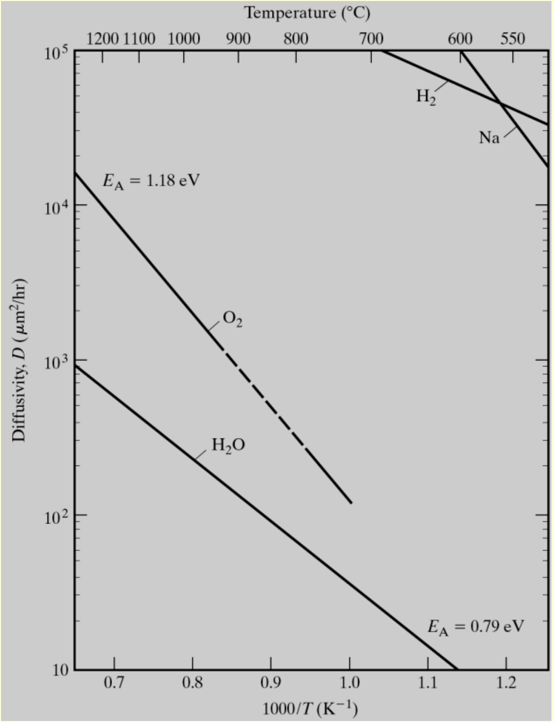


FIGURE 3.1

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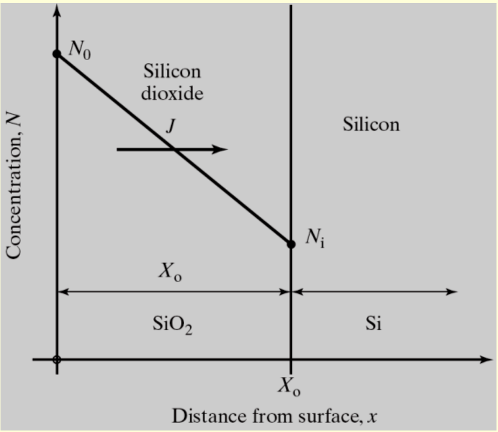


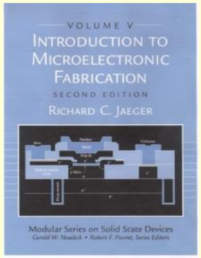
$$D = D_O \exp\left(-\frac{E_A}{kT}\right)$$ Arrhenius Relationship

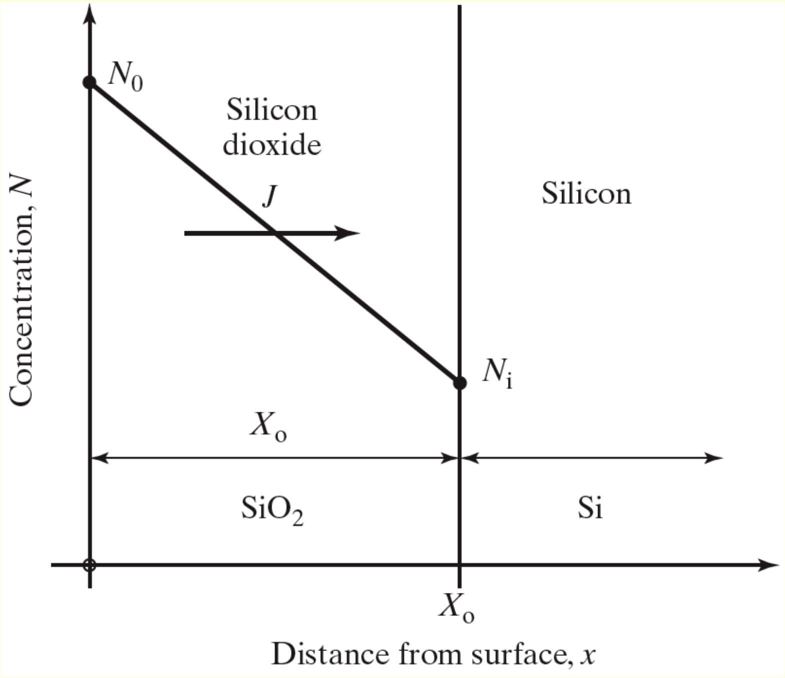
E_A = activation energy

k = Boltzmann's constant = 1.38×10^{-23} J/K

T = absolute temperature

Thermal Oxidation
Oxidation Theory





$$J = -D\frac{\partial N(x,t)}{\partial x} = -D\frac{(N_i - N_0)}{X_O}$$

$$J(X_o) = k_s N_i$$

$$t = \frac{X_o^2}{B} + \frac{X_o}{(B/A)} - \tau \qquad \tau = \frac{X_i^2}{B} + \frac{X_i}{(B/A)}$$

$$A = \frac{2D}{k_s} \qquad B = \frac{2DN_0}{M}$$

$$X_o(t) = 0.5A\left[\left\{1 + 4\frac{B}{A^2}(t+\tau)\right\}^{0.5} - 1\right]$$

Oxide growth occurs at X_o

X_o = final oxide thickness

X_i = initial oxide thickness

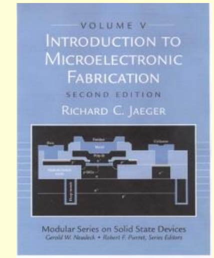
τ = time required to grow initial oxide

D = diffusion coefficient

N = concentration of oxygen

k_s = rate constant at $S_i - S_iO_2$ interface

Oxidation Theory
Parabolic Regime



For Long Times - $(t+\tau) >> \frac{A^2}{4B}$

$$X_o(t) = \sqrt{Bt}$$

B = parabolic rate constant

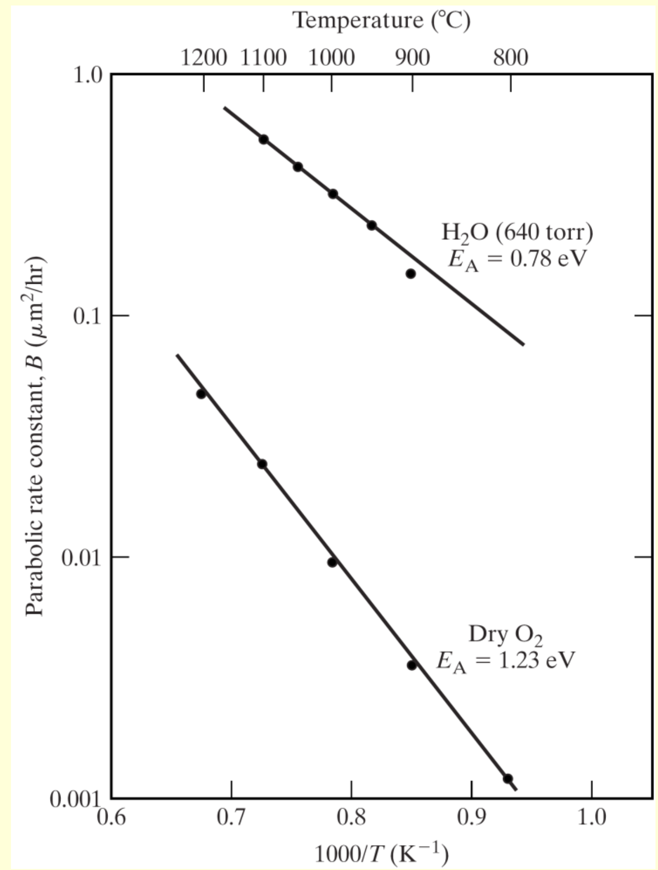


FIGURE 3.4

Dependence of the parabolic rate constant B on temperature for the thermal oxidation of silicon in pyrogenic H_2O (640 torr) or dry O_2. Reprinted by permission of the publisher, The Electrochemical Society, Inc., from Ref. [10].

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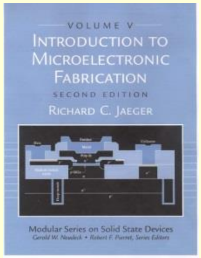
Oxidation Theory
Linear Regime



For Short Times - $(t+\tau) << \dfrac{A^2}{4B}$

$$X_o(t) \cong \left(\frac{B}{A}\right)(t+\tau)$$

$$\left(\frac{B}{A}\right) = \text{linear rate constant}$$

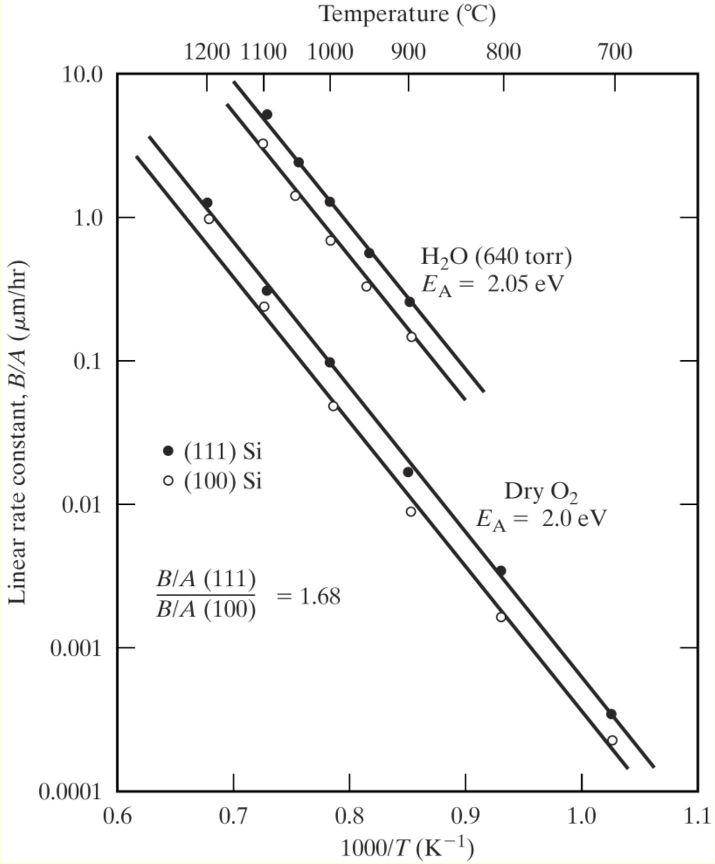


FIGURE 3.5

Dependence of the linear rate constant B/A on temperature for the thermal oxidation of silicon in pyrogenic H_2O (640 torr) or dry O_2. Reprinted by permission of the publisher, The Electrochemical Society, Inc., from Ref. [10].

Rate Constants
Wet and Dry Oxidation

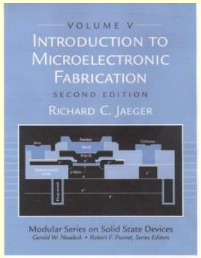


TABLE 3.1 Values for Coefficient D_0 and Activation Energy E_A for Wet and Dry Oxygen*

	Wet O_2(X_i = 0 nm)		Dry O_2(X_i = 25 nm)	
	D_0	E_A	D_0	E_A
<100> Silicon				
Linear (B/A)	9.70×10^7 μm/hr	2.05 eV	3.71×10^6 μm/hr	2.00 eV
Parabolic (B)	386μm^{2}}/hr	0.78 eV	772μm^2/hr	1.23 eV
<111> Silicon				
Linear (B/A)	1.63×10^8 μm/hr	2.05 eV	6.23μ10^6 μm/hr	2.00 eV
Parabolic (B)	386μm^2/hr	0.78 eV	772μm^2/hr	1.23 eV

*Data from Ref.[9]

- Wet oxidation is much more rapid than dry oxidation
- Note that dry oxidation appears to always have some initial oxide present
- Dry oxidation (slow) produces higher quality oxide than wet oxidation

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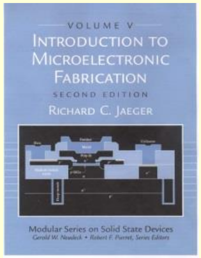
Thermal Oxidation
Oxidation on <100> Silicon



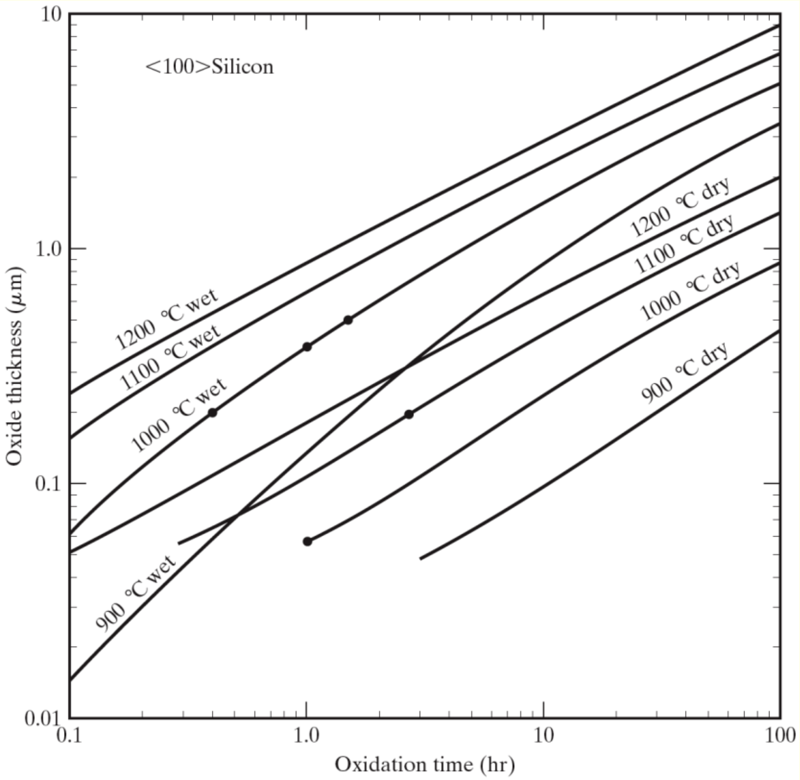


FIGURE 3.6

Wet and dry silicon dioxide growth for <100> silicon calculated using the data from Table 3.1. (The dots represent data used in examples.)

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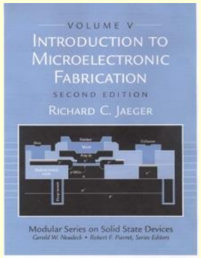
Thermal Oxidation
Oxidation on <111> Silicon



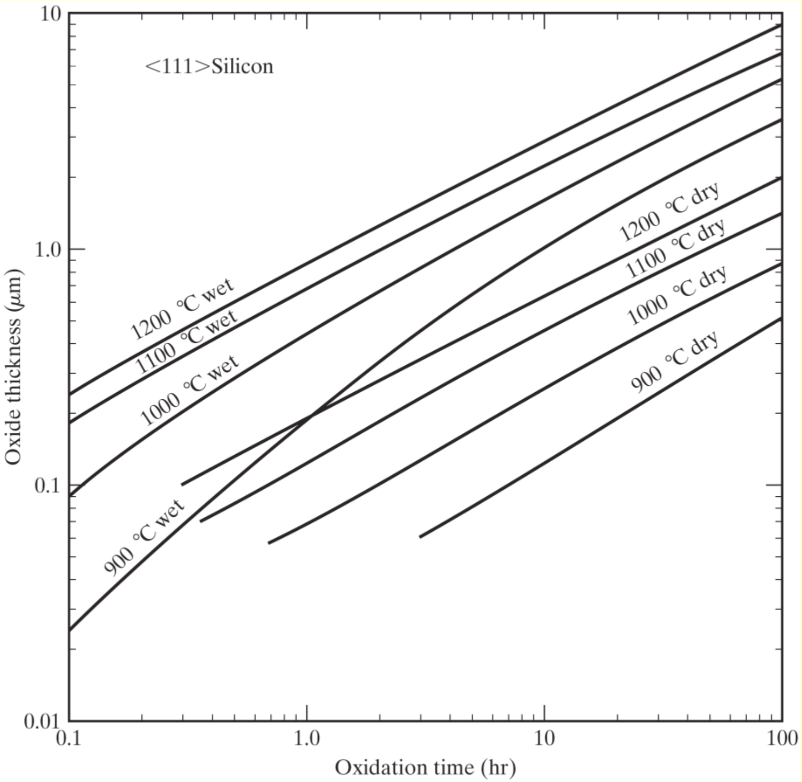
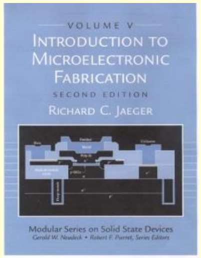


FIGURE 3.7

Wet and dry silicon dioxide growth for <111> silicon calculated using the data from Table 3.1.

Thermal Oxidation Example



Example 3.2

A <100> wafer has a 2000-Å oxide on its surface.

(a) How long did it take to grow this oxide at 1100 °C in dry oxygen?

(b) The wafer is put back in the furnace in wet oxygen at 1000 °C. How long will it take to grow an additional 3000 Å of oxide? Solve this problem graphically using Figs. 3.6 and 3.7 as appropriate.

(c) Repeat part (b) using the oxidation theory presented in Eqs. (3.3) through (3.12).

Solution: **(a)** According to Fig. 3.6, it would take 2.8 hr to grow a 0.2-μm oxide in dry oxygen at 1100 °C.

(b) We can solve part (b) graphically using Fig. 3.6. The total oxide at the end of the oxidation would be 0.5 μm. If there were no oxide on the surface, it would take 1.5 hr to grow 0.5 μm. However, there is already a 0.2μm oxide on the surface, and the wafer "thinks" that it has already been in the furnace for 0.4 hr. The time required to grow the additional 0.3 μm of oxide is the difference in these two times: $\Delta t = (1.5 - 0.4)$ hr $= 1.1$ hr.

(c) From Table 3.1, $B = 3.86 \times 10^{2} \exp(-0.78/kT)$ μm^{2}/hr and $(B/A) = 0.97 \times 10^{8} \exp(-2.05/kT)$ μm/hr. Using T = 1,273 K and $k = 8.617 \times 10^{-5}$ eV/Kg, $B = 0.314$ $\mu m^{2} \times$ /hr and $(B/A) = 0.738$ μm/hr. Using these values and an initial oxide thickness of 0.2m yields a value of 0.398 hr for the effective initial oxidation time τ. Using τ and a final oxide thickness of 0.5 μm yields an oxidation time of 1.08 hr. Note that both the values of t and τ are close to those found in part (b). Of course, the graphical results depend on our ability to interpolate logarithmic scales!

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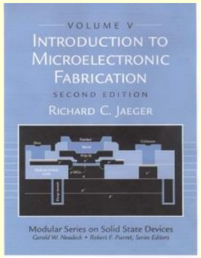


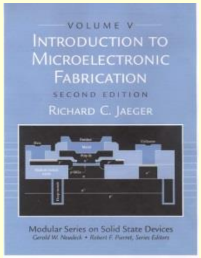
Thermal Oxidation Example

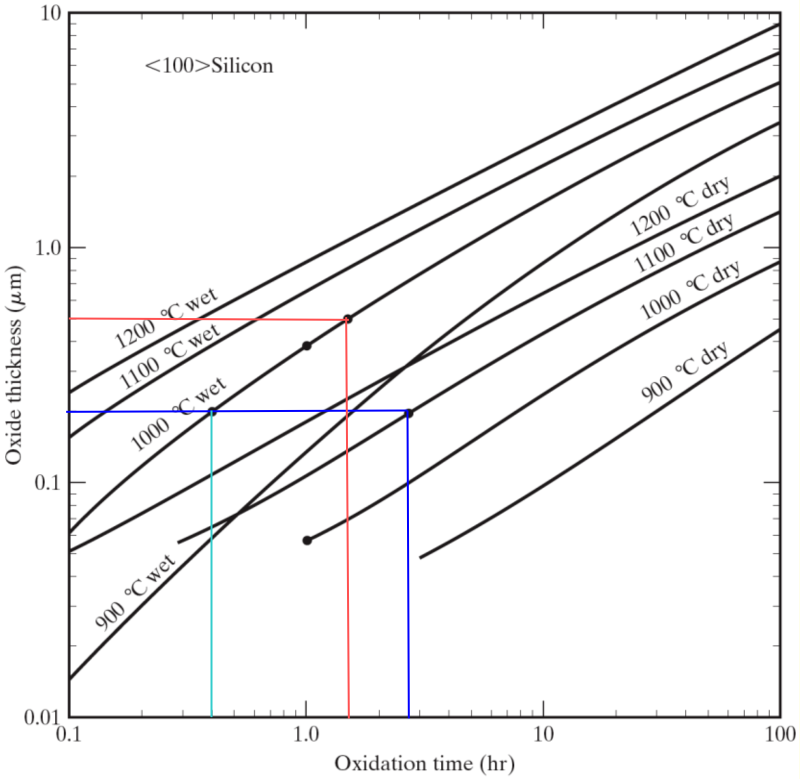
A <100> silicon wafer has a 2000-Å oxide on its surface

(a) How long did it take to grow this oxide at 1100^{o} C in dry oxygen?

(b)The wafer is put back in the furnace in wet oxygen at 1000^{o} C. How long will it take to grow an additional 3000 Å of oxide?

Thermal Oxidation Example
Graphical Solution

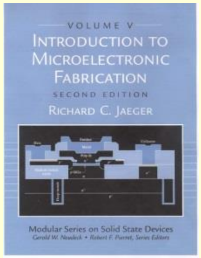




(a) According to Fig. 3.6, it would take 2.8 hr to grow 0.2 μm oxide in dry oxygen at 1100° C.

(b) The total oxide thickness at the end of the oxidation would be 0.5 μm which would require 1.5 hr to grow if there was no oxide on the surface to begin with. However, the wafer "thinks" it has already been in the furnace 0.4 hr. Thus the additional time needed to grow the 0.3 μm oxide is 1.5-0.4 = 1.1 hr.

Thermal Oxidation Example
Mathematical Solution



(a) From Table 3.1,

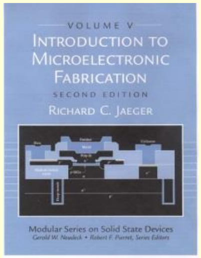
$$B = 7.72x10^2 \exp\left(\frac{-1.23}{kT}\right)\frac{\mu m^2}{hr} \qquad \frac{B}{A} = 3.71x10^6 \exp\left(\frac{-2.00}{kT}\right)\frac{\mu m}{hr} \qquad X_i = 25nm$$

For T = 1273 K, $B = 0.0236\,\frac{\mu m^2}{hr}$ and $\frac{B}{A} = 0.169\,\frac{\mu m}{hr}$

$$\tau = \frac{(0.025\mu m)^2}{0.0236\,\frac{\mu m^2}{hr}} + \frac{0.025\mu m}{0.169\,\frac{\mu m}{hr}} = 0.174\ hr$$

$$t = \frac{(0.2\mu m)^2}{0.0236\,\frac{\mu m^2}{hr}} + \frac{0.2\mu m}{0.169\,\frac{\mu m}{hr}} - 0.174\,hr = 2.70\ hr$$

Thermal Oxidation Example
Mathematical Solution



(b) From Table 3.1,

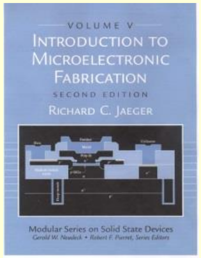
$$B = 3.86x10^2 \exp\left(\frac{-0.78}{kT}\right)\frac{\mu m^2}{hr} \qquad \frac{B}{A} = 9.70x10^7 \exp\left(\frac{-2.05}{kT}\right)\frac{\mu m}{hr} \qquad X_i = 0$$

For $\mathrm{T} = 1273\ \mathrm{K}$, $\mathrm{B} = 0.314\,\frac{\mu m^2}{hr}$ and $\frac{B}{A} = 0.742\,\frac{\mu m}{hr}$

$$\tau = \frac{(0.2\mu m)^2}{0.314\,\frac{\mu m^2}{hr}} + \frac{0.2\mu m}{0.742\,\frac{\mu m}{hr}} = 0.398\ hr$$

$$t = \frac{(0.5\mu m)^2}{0.314\,\frac{\mu m^2}{hr}} + \frac{0.5\mu m}{0.742\,\frac{\mu m}{hr}} - 0.398 hr = 1.07\ hr$$

Thermal Oxidation
Wet High Pressure Oxidation



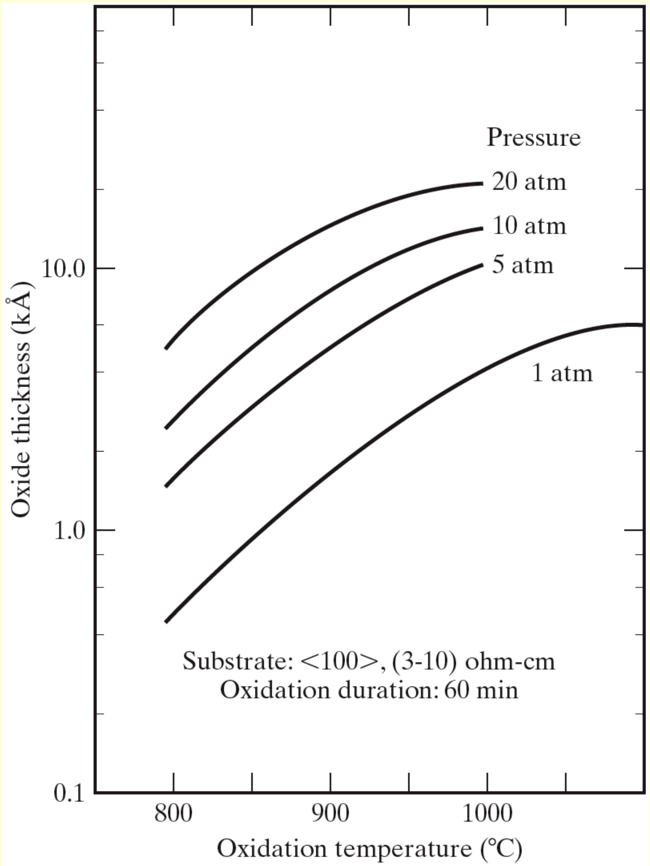
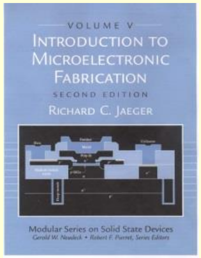


FIGURE 3.8

Wet oxide growth at increased pressures. Reprinted with permission of Solid State Technology, published by Technical Publishing, a company of Dun and Bradstreet, from Ref. [12].

Thermal Oxidation Impurity Redistribution



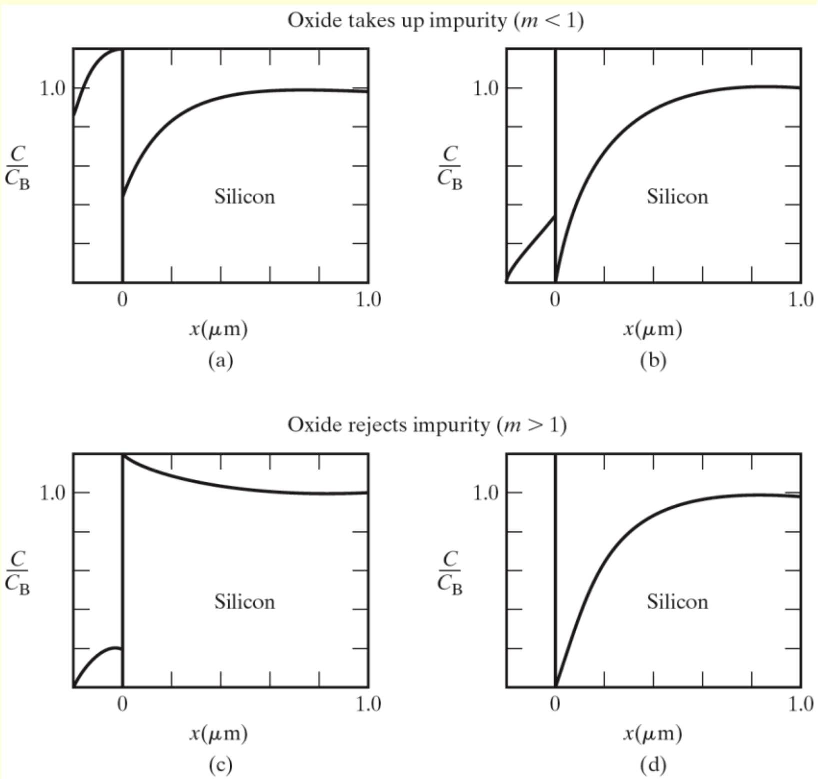
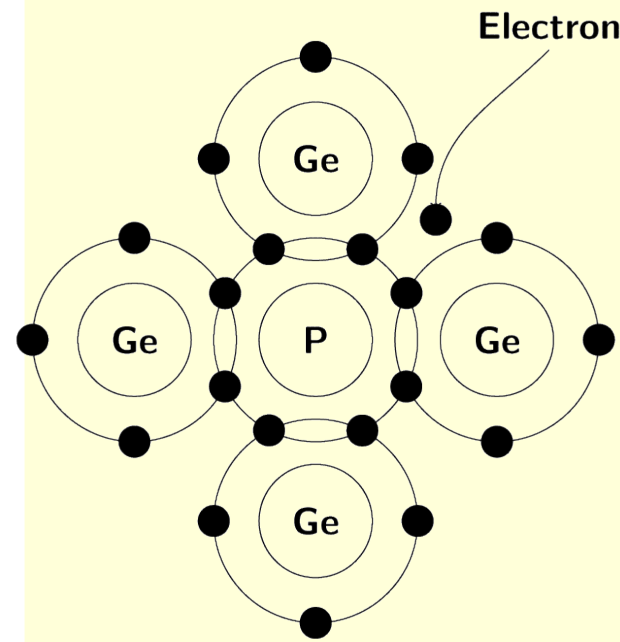


FIGURE 3.9

The effects of oxidation on impurity profiles. (a) Slow diffusion in oxide (boron); (b) fast diffusion in oxide (boron with hydrogen ambient); (c) slow diffusion in oxide (phosphorus); (d) fast diffusion in oxide (gallium). C_B is the bulk concentration in the silicon. Copyright John Wiley & Sons, Inc. Reprinted with permission from Ref. [5].

$$m = \frac{dopant\ concentration\ in\ Si}{dopant\ concentration\ in\ SiO_2}$$



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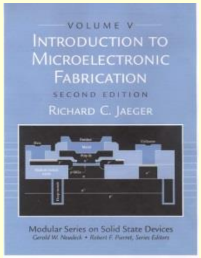
Thermal Oxidation Masking Properties of SiO_2



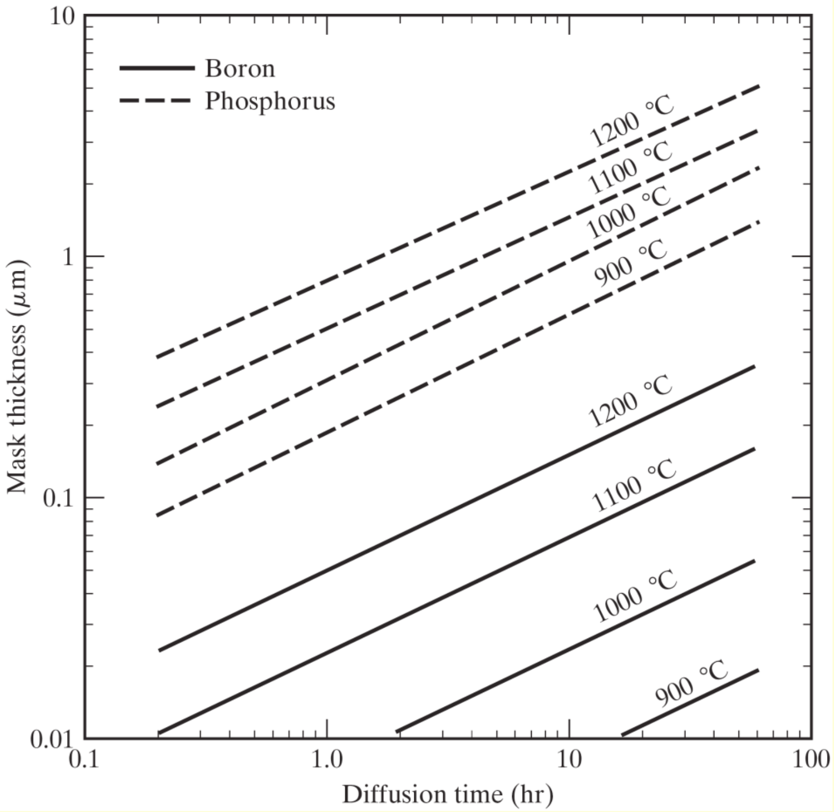
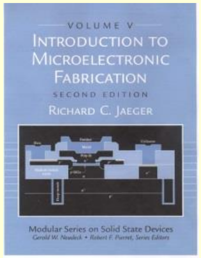


FIGURE 3.10

Thickness of silicon dioxide needed to mask boron and phosphorus diffusions as a function of diffusion time and temperature.

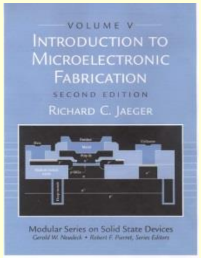
- Required oxide thickness depends upon dopant species and temperature
- Hydrogen greatly enhances diffusion of boron - wet oxidation release hydrogen

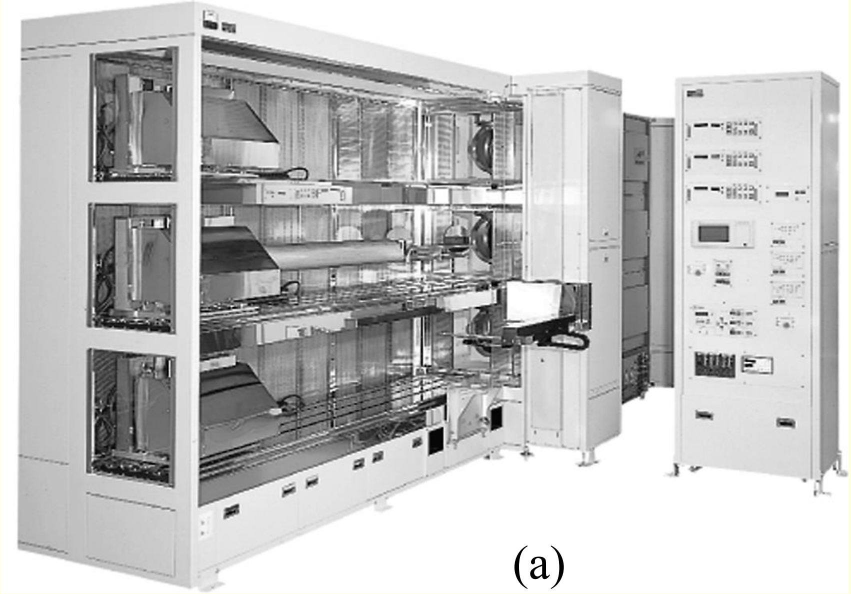
Thermal Oxidation
Oxide Quality



- Dry oxidation (slow) produces higher quality oxide than wet oxidation
- Oxidations often consist of sequence of dry-wet-dry oxidation cycles -Most of oxide is grown during wet phase
- Dry phase yields higher density oxide with improved breakdown voltage (5-10 MV/cm)
- Dry oxidation usually used to grow gate oxides
- Nitrogen being added to form oxynitrides for very thin gate oxides

Thermal Oxidation
Oxidation Systems






(b)

Figure 3.11 Furnaces used for oxidation and diffusion
(a) A three-tube horizontal furnace with multizone temperature control
(b) Vertical furnace (Courtesy of Crystec, Inc.)

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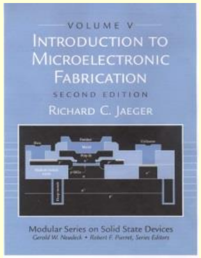
Local Oxidation of Silicon (LOCOS)



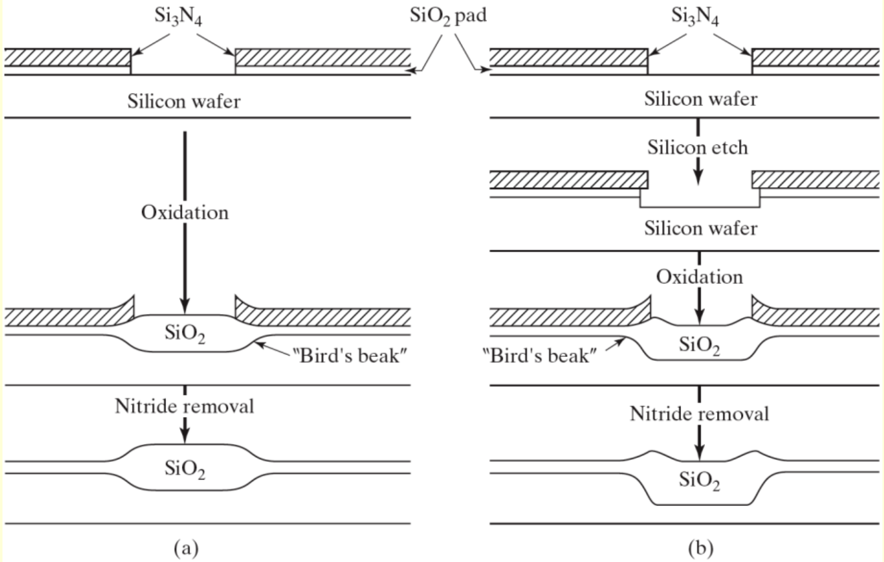


FIGURE 3.12

Cross section depicting process sequence for local oxidation of silicon (LOCOS): (a) semirecessed and (b) fully recessed structures.

- Isolation technology in MOS processes
- Provides isolation between nearby devices
- Fully recessed process attempts to minimize bird's beak

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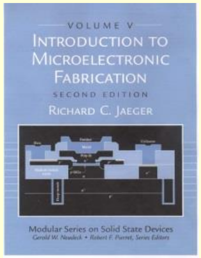
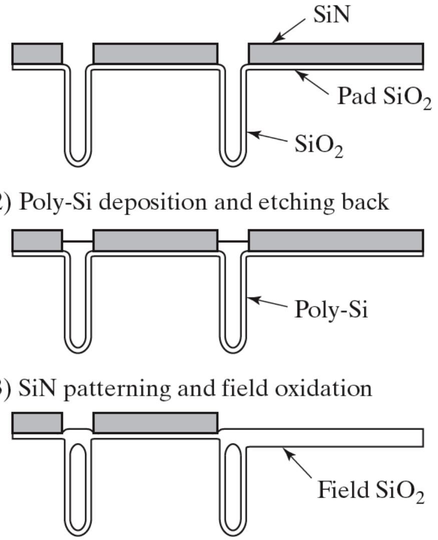
Thermal Oxidation
Deep Trench Isolation





Fabrication procedure of trench isolation and field oxide.

(a) Deep-trench process

FIGURE 3.13

Trench isolation structures. (a) Deep trench isolation - Copyright 1996 IEEE. Reprinted with permission from Ref. [18]. (b) Shallow trench isolation - Copyright 1998 IEEE. Reprinted with permission from Ref. [20].

- Often used in dynamic memory chips (DRAMS)
- Deep trenches used in high performance bipolar processes

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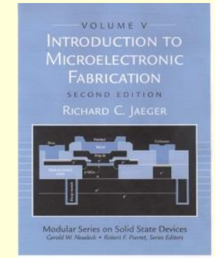
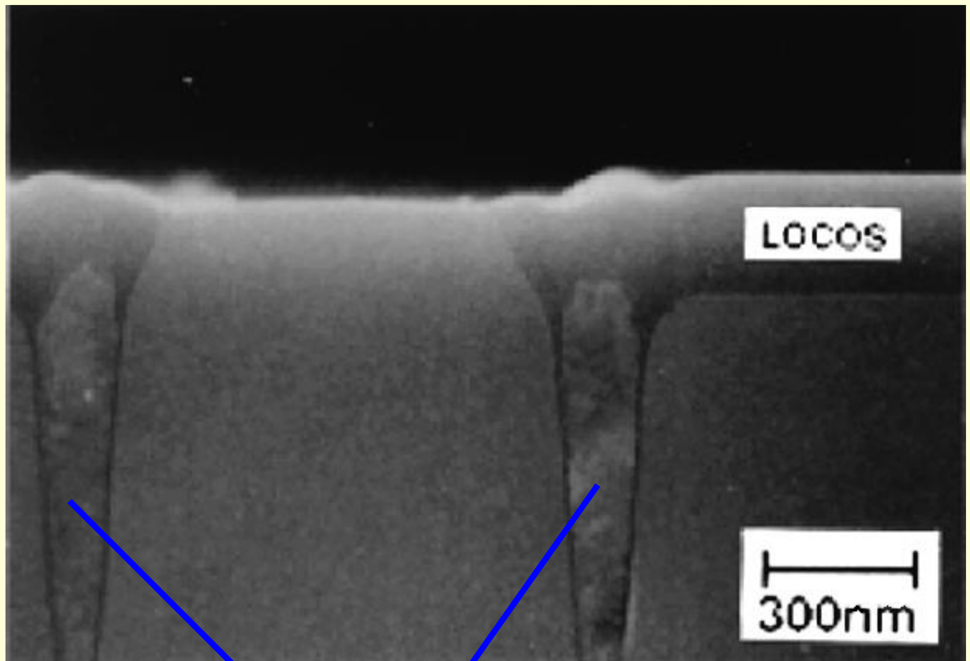
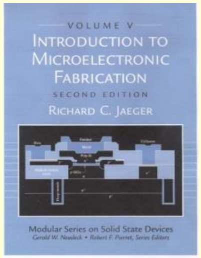
Thermal Oxidation
Example of Deep Trenches





Filled Trenches

Thermal Oxidation
Shallow Trench Isolation



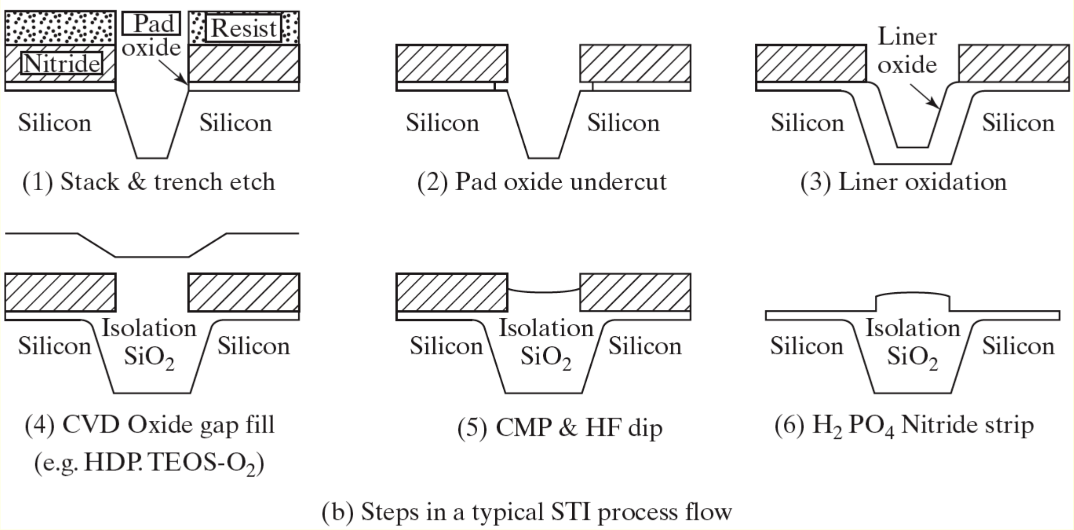
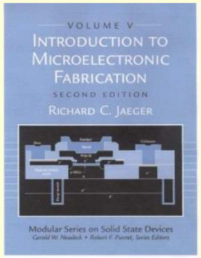


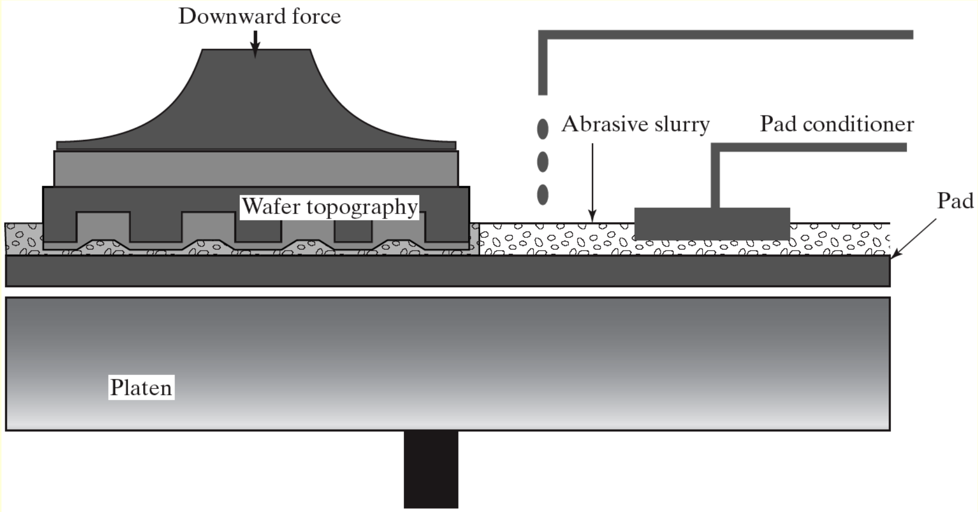
FIGURE 3.13

Trench isolation structures. (a) Deep trench isolation - Copyright 1996 IEEE. Reprinted with permission from Ref. [18]. (b) Shallow trench isolation - Copyright 1998 IEEE. Reprinted with permission from Ref. [20].

Used for isolation between devices and to minimize device capacitance

Chemical Mechanical Polishing (CMP)





- Mechanical polishing is widely used to achieve highly planar surfaces
- Used in multilevel metalization systems including both aluminum and copper

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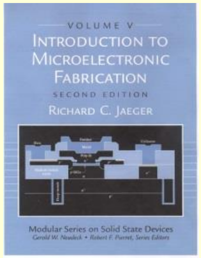
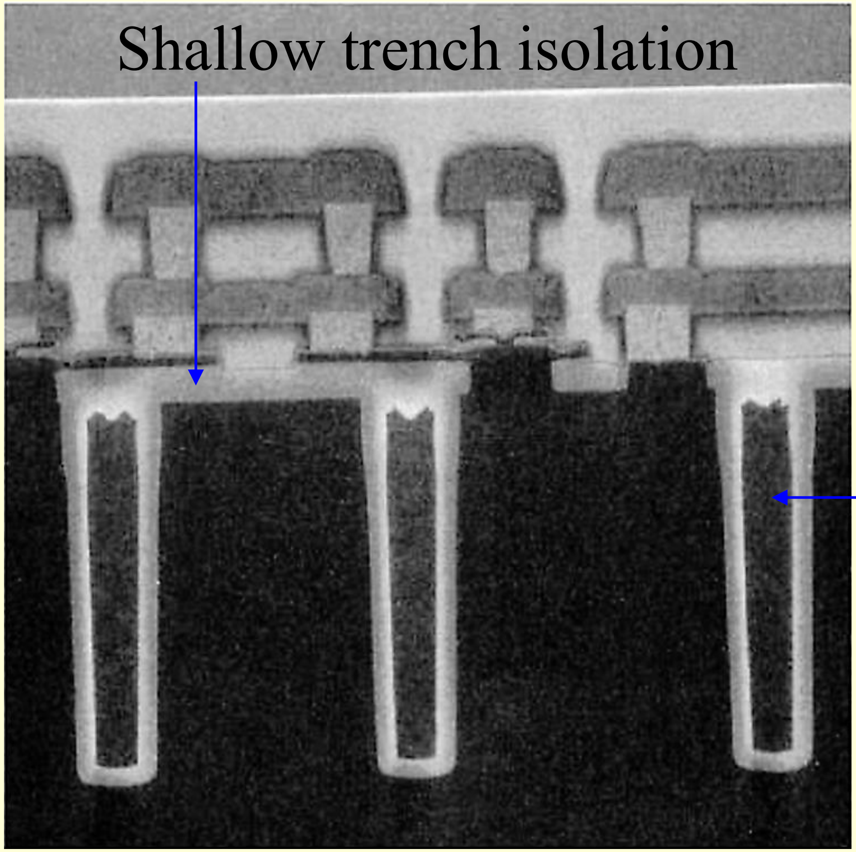
Thermal Oxidation Trench Isolation Example



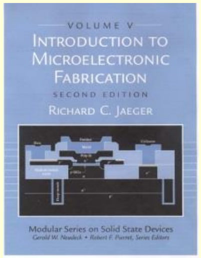


CMP planarization

Deep trench isolation

Figure 3.14 Microphotograph of actual deep and shallow trench isolation applied to SiGE HBT technology. Copyright 1998 IEEE. Reprinted with permission from Ref. [31].

Multilevel Metallization Using CMP



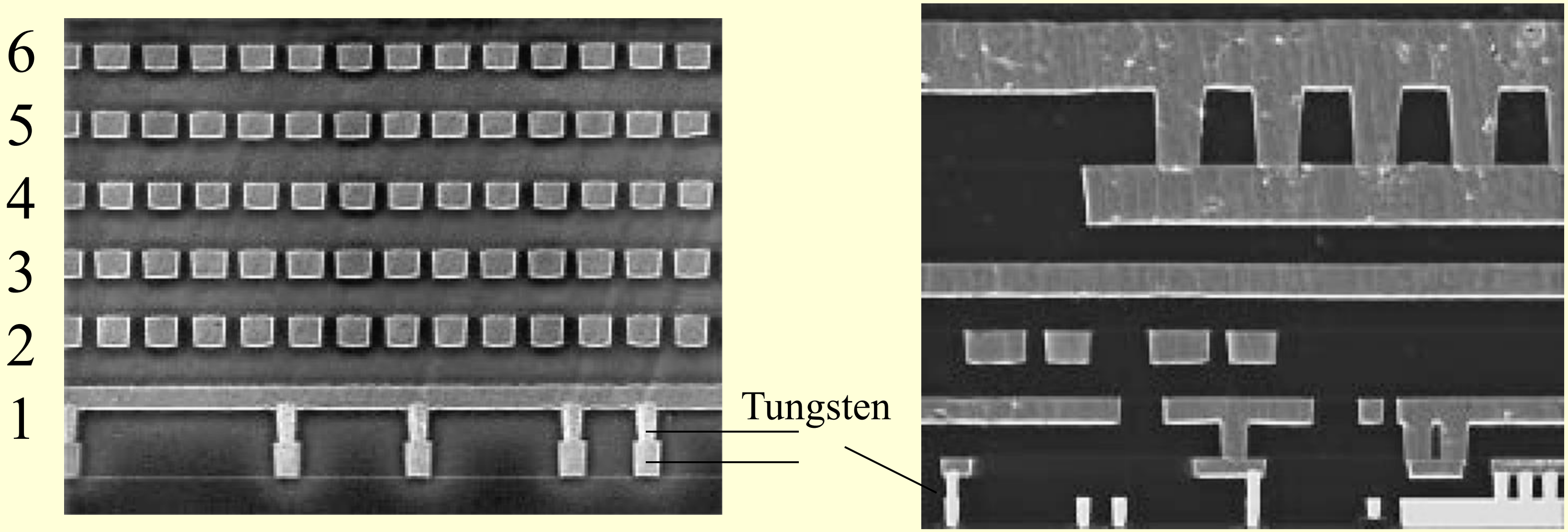


Figure 3.16 Multilevel metallization fabricated with chemical mechanical polishing (a) SEM of 6-level thin-wire copper. First-level copper is connected with tungsten studs to tungsten local interconnect. (b) SEM of 6-level copper with low RC metallization on levels 5 and 6. Copyright 1997 IEEE. Reprinted with permission from Ref. [24].

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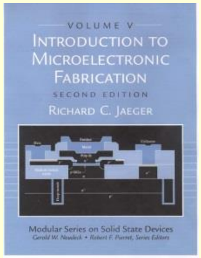
Oxide Thickness Determination

TABLE 3.2 Color Chart for Thermally Grown SiO_2 Films Observed Perpendicularly Under Daylight Fluorescent Lighting. Copyright 1964 by International Business Machines Corporation; reprinted with permission from Ref. [11].

Film Thickness (μm)	Color and Comments	Film Thickness (μm)	Color and Comments
0.05	Tan	0.58	Light orange or yellow to pink
0.07	Brown	0.60	Carnation pink
0.10	Dark violet to red violet	0.63	Violet red
0.12	Royal blue	0.68	"Bluish" (not blue but borderline between violet and blue green; appears more like a mixture between violet red and blue green and looks grayish)
0.15	Light blue to metallic blue	0.72	Blue green to green (quite broad)
0.17	Metallic to very light yellow green	0.77	"Yellowish"
0.20	Light gold or yellow; slightly metallic	0.80	Orange (rather broad for orange)
0.22	Gold with slight yellow orange	0.82	Salmon
0.25	Orange to melon	0.85	Dull, light red violet
0.27	Red violet	0.86	Violet
0.30	Blue to violet blue	0.87	Blue violet
0.31	Blue	0.89	Blue
0.32	Blue to blue green	0.92	Blue green
0.34	Light green	0.95	Dull yellow green
0.35	Green to yellow green	0.97	Yellow to "yellowish"
0.36	Yellow green	0.99	Orange
0.37	Green yellow	1.00	Carnation pink
0.39	Yellow	1.02	Violet red
0.41	Light orange	1.05	Red violet
0.42	Carnation pink	1.06	Violet
0.44	Violet red	1.07	Blue violet
0.46	Red violet	1.10	Green
0.47	Violet	1.11	Yellow green
0.48	Blue violet	1.12	Green
0.49	Blue	1.18	Violet
0.50	Blue green	1.19	Red violet
0.52	Green (broad)	1.21	Violet red
0.44	Violet red	1.24	Carnation pink to salmon
0.46	Red violet	1.25	Orange
0.47	Violet	1.28	"Yellowish"
0.48	Blue violet	1.32	Sky blue to green blue
0.49	Blue	1.40	Orange
0.50	Blue green	1.45	Violet
0.52	Green (broad)	1.46	Blue violet
0.54	Yellow green	1.50	Blue
0.56	Green yellow	1.54	Dull yellow green
0.57	Yellow to "yellowish" (not yellow but is in the position where yellow is to be expected; at times appears to be light creamy gray or metallic)		



- Oxide Color Chart

Oxide thickness for constructive interference

$$2X_o = \frac{k\lambda}{n}$$

n = index of refraction (1.46 for SiO_2)

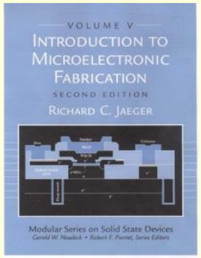
$k \in [1, 2, 3, ...]$

- Ellipsometer - direct measurement

Oxide Thickness Determination

SiO_2 Thickness Color Chart

Film Thickness (Å)	Color of Film (those shown are only indicative)
500	tan
700	brown
1000	dark violet to red violet
1200	royal blue
1500	light blue to metallic blue
1700	metallic to very light yellow-green
2000	light gold or yellow - slightly metallic
2200	gold with slight yellow-orange
2500	orange to melon
2700	red-violet
3000	blue to violet-blue
3100	blue
3200	blue to blue-green
3400	light green
3500	green to yellow-green
3600	yellow-green
3700	green-yellow
3900	yellow
4100	light orange
4200	carnation pink
4400	violet-red
4600	red-violet
4700	violet
4800	blue-violet
4900	blue
5000	blue-green
5200	green
5400	yellow-green
5600	green-yellow
5700	yellow to "yellowish" (at times appears light gray or metallic)
5800	light orange or yellow to pink
6000	carnation pink
6300	violet-red
6800	"bluish" (appears between violet-red and blue-green - overall looks grayish
7200	blue-green to green
7700	"yellowish"
8000	orange
8200	salmon
8500	dull light red-violet
8600	violet
8700	blue-violet
8900	blue
9200	blue-green
9500	dull yellow-green
9700	yellow to "yellowish"
9900	orange



- Oxide Color Chart

Oxide thickness for constructive interference

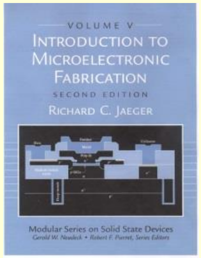
$$2X_o = \frac{k\lambda}{n}$$

n = index of refraction (1.46 for SiO_2)

$k \in [1, 2, 3, ...]$

- Ellipsometer - direct measurement

Process Simulation
SUPREM Oxidation Example



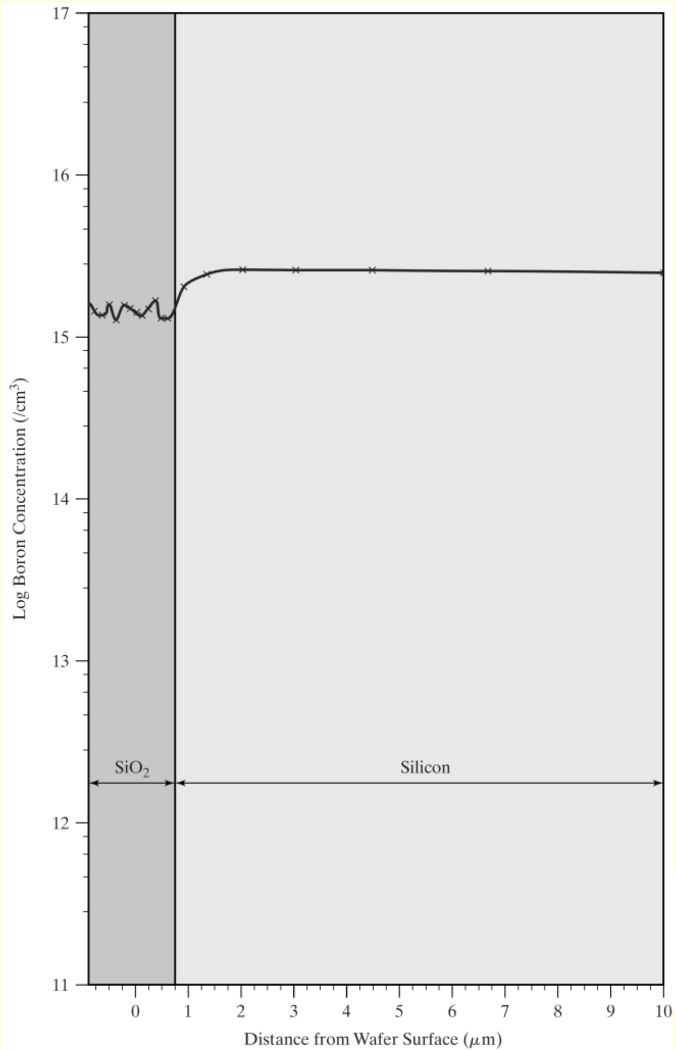


FIGURE 3.17

Results of SUPREM simulation of oxide growth on boron doped silicon wafers.

SUPREM
Stanford University Process Engineering Modeling Program [25-27]

http://www-tcad.stanford.edu/

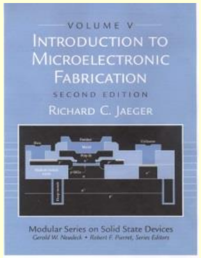
TABLE 3.3 SUPREM-IV Simulation Example

```
$ Multistep Oxidation

$ Use Automatic Grid Generation and Adaptive Grid

INITIALIZE <100> BORON = 5 RESISTIV
DIFFUSION TEMP=950 TIME=30 F.N2 = 5
DIFFUSION TEMP=950 TIME=30 T.FINAL = 1100 F.O2 = 5
DIFFUSION TEMP=1100 TIME=300 STEAM
DIFFUSION TEMP=1100 TIME=60 F.O2 = 5
DIFFUSION TEMP=1100 TIME=60 T.FINAL = 800 F.N2 = 5
$ Print layer information
....
....
$ Plot results
....
....
```

Thermal Oxidation References



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End of Chapter 3

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