# Introduction to Microelectronic Fabrication


by

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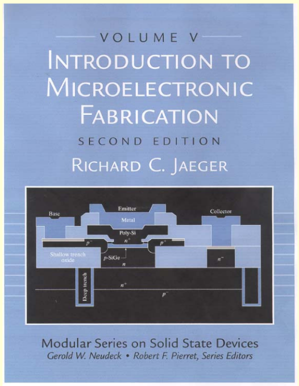
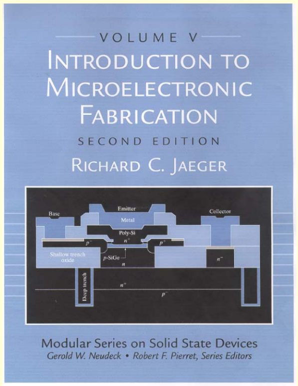



## Chapter 3

## Thermal Oxidation of Silicon







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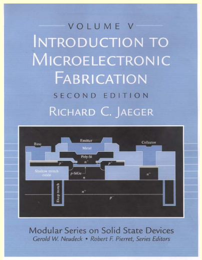


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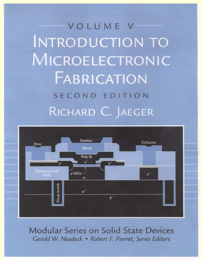
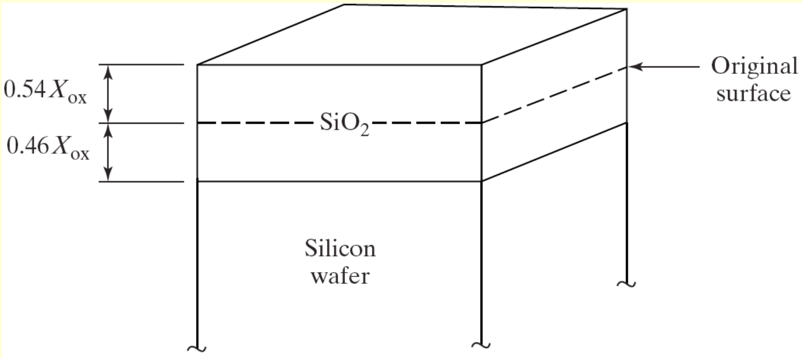
# Thermal Oxidation of Silicon




•Silicon Dioxide

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




Dry Oxidation

$$S_i + O_2 \rightarrow S_iO_2$$

Wet Oxidation

$$S_i + 2H_2O \rightarrow S_iO_2 + 2H_2$$

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



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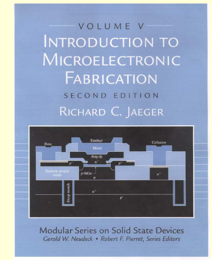
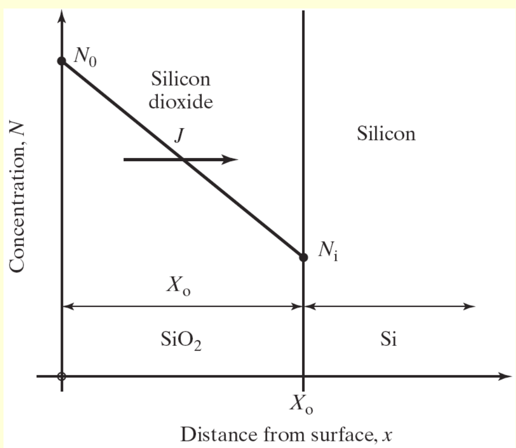
# Thermal Oxidation
# Fick's First Law of Diffusion




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

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

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



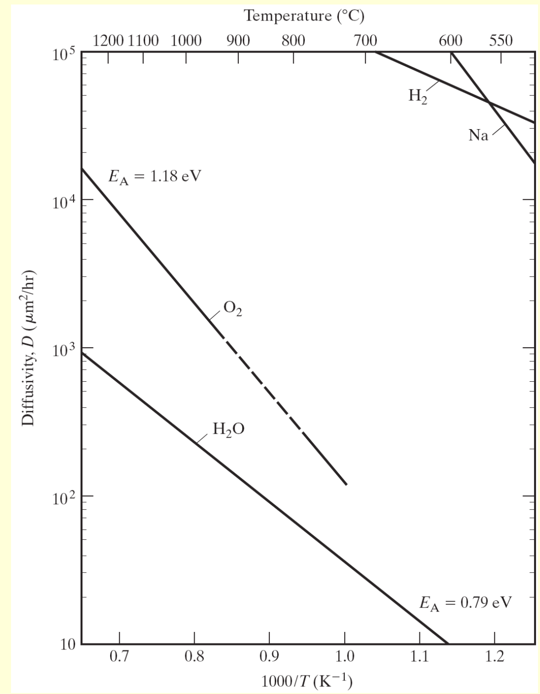
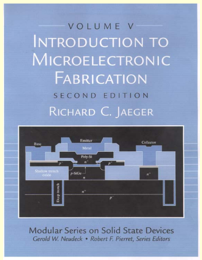




FIGURE 3.1

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

# Thermal Oxidation
# Fick's First Law of Diffusion



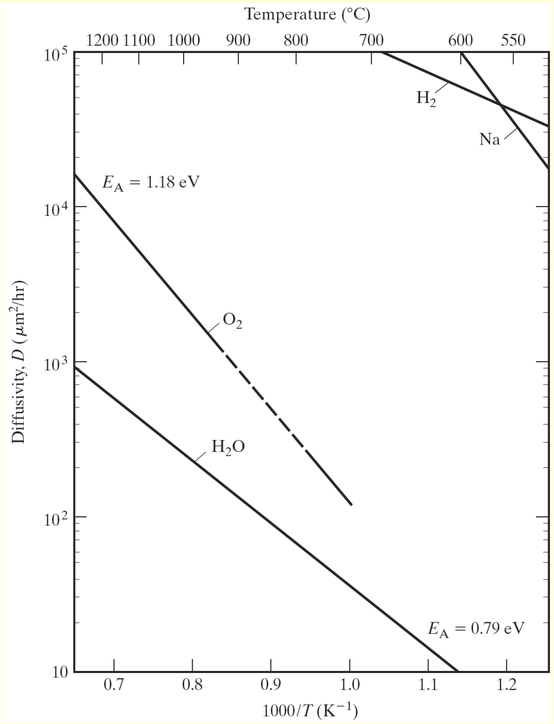
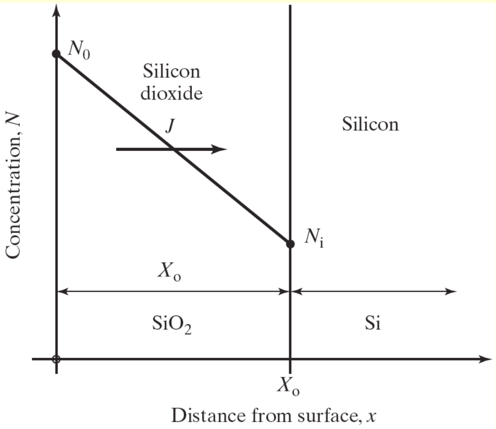




FIGURE 3.1

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




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

$E_A$ = activation energy

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

T = absolute temperature



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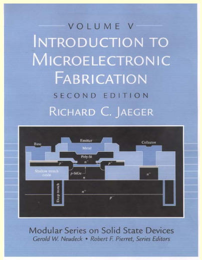
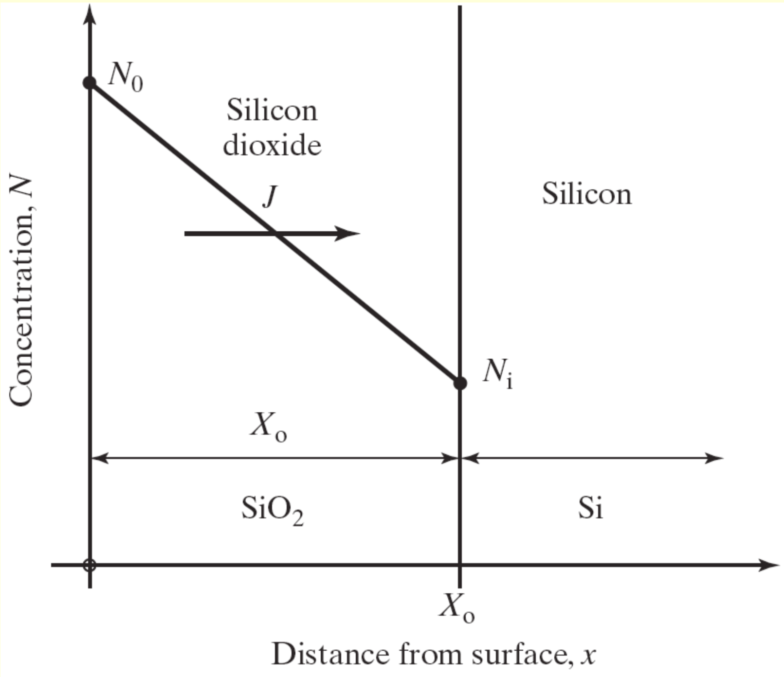
# Thermal Oxidation
# Oxidation Theory




Oxide growth occurs at $X_o$

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

$$J(X_o) = k_s N_i$$

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

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

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

$X_o$ = final oxide thickness

$X_i$ = initial oxide thickness

$\tau$ = time required to grow initial oxide

$D$ = diffusion coefficient

$N$ = concentration of oxygen

$k_s$ = rate constant at $S_i - S_iO_2$ interface



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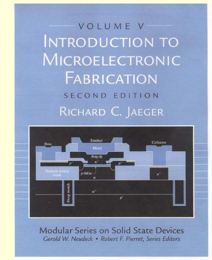
# Oxidation Theory

## Parabolic Regime




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

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

B = parabolic rate constant

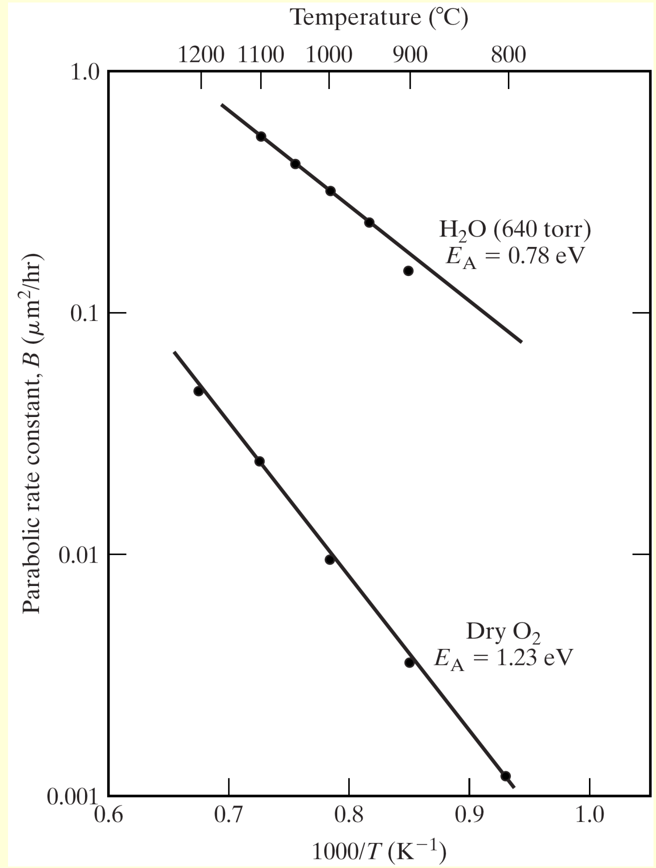



FIGURE 3.4

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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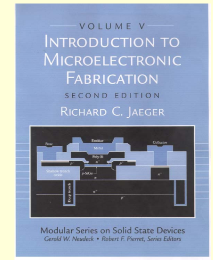
# Oxidation Theory
## Linear Regime




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

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

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

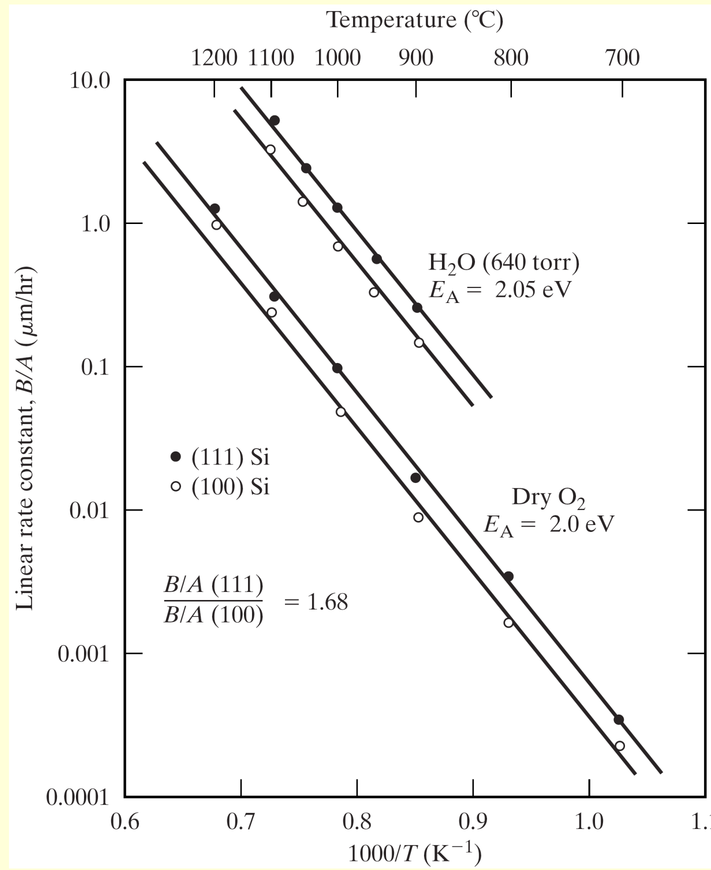



FIGURE 3.5

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].



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# Rate Constants

## Wet and Dry Oxidation

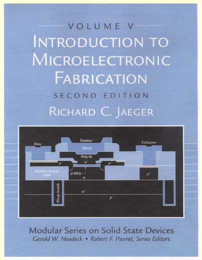


TABLE 3.1 Values for Coefficient $D_0$ and Activation Energy $E_A$ for Wet and Dry Oxygen*

| | 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) | $9.70 \times 10^{7}$ $\mu$m/hr | 2.05 eV | $3.71 \times 10^{6}$ $\mu$m/hr | 2.00 eV |
| Parabolic (B) | $386\mu m^{2}$/hr | 0.78 eV | $772\mu m^{2}$/hr | 1.23 eV |
| <111> Silicon | | | | |
| Linear (B/A) | $1.63 \times 10^{8}$ $\mu$m/hr | 2.05 eV | $6.23\mu 10^{6}$ $\mu$m/hr | 2.00 eV |
| Parabolic (B) | $386\mu m^{2}$/hr | 0.78 eV | $772\mu m^{2}$/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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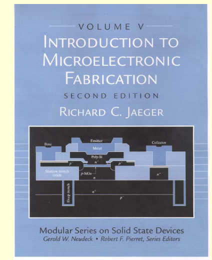
# Thermal Oxidation
# Oxidation on <100> Silicon



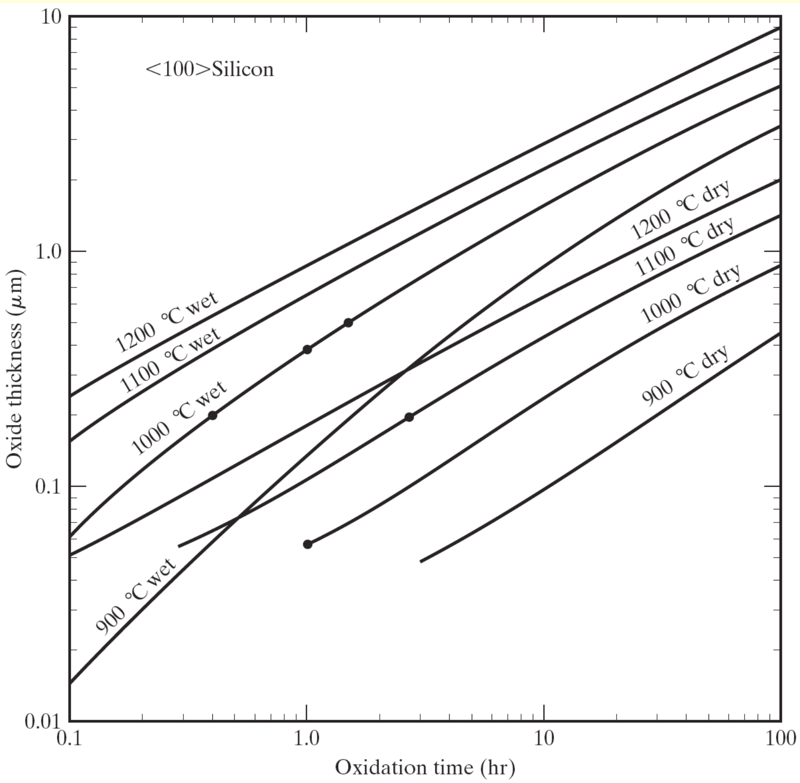




FIGURE 3.6

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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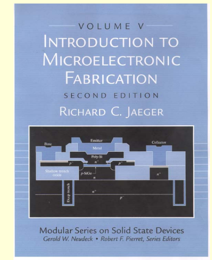
# Thermal Oxidation
# Oxidation on <111> Silicon



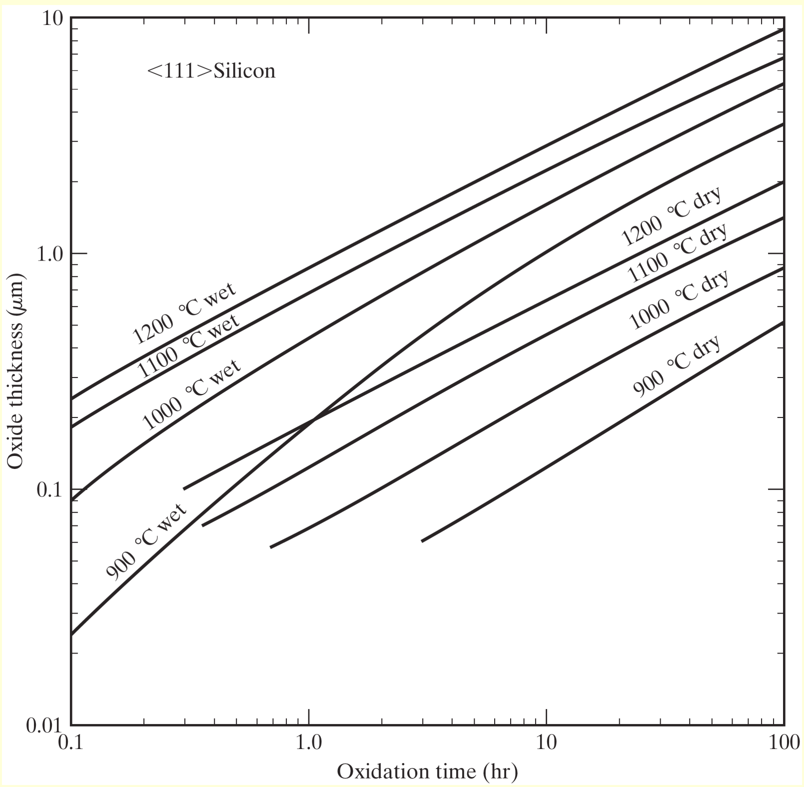




FIGURE 3.7

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



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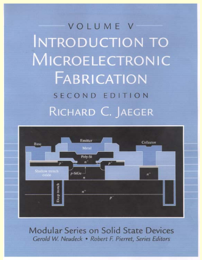
# Thermal Oxidation Example




**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 $k = 8.617 \times 10^{-5}$ $e$V/Kg, $B = 0.314$ μm$^2$ × /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 $\tau$. Using $\tau$ 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 $\tau$ 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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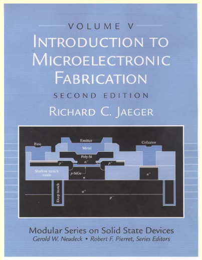
# Thermal Oxidation Example

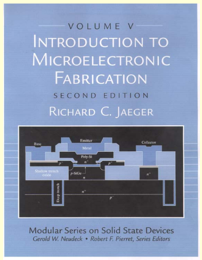


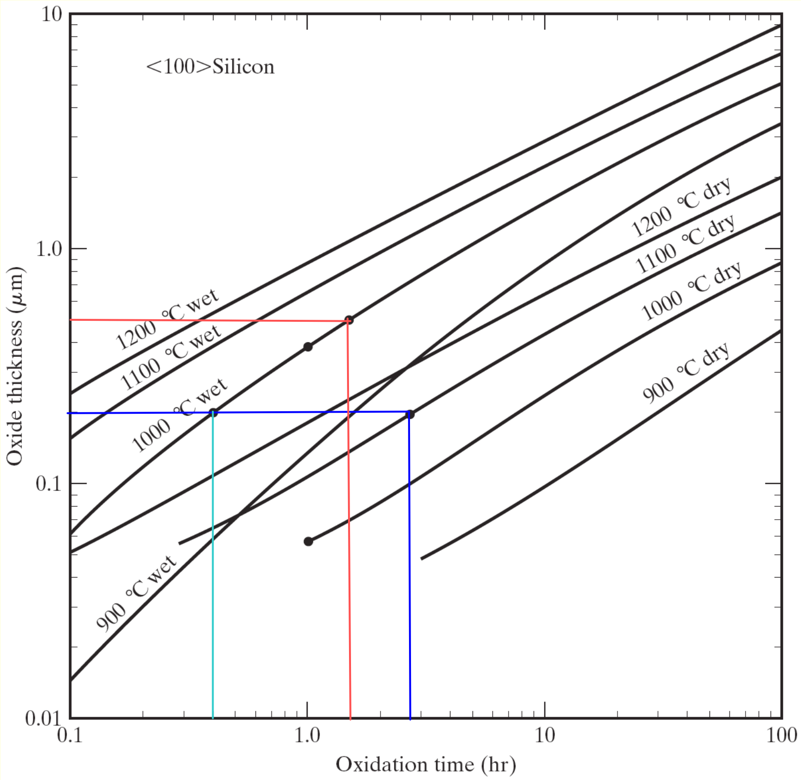

A <100> silicon wafer has a 2000-Å oxide on its surface

(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.



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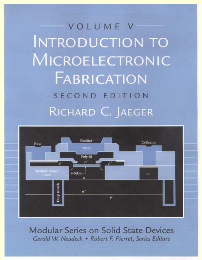
# Thermal Oxidation Example
## Mathematical Solution




(a) From Table 3.1,

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

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

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

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



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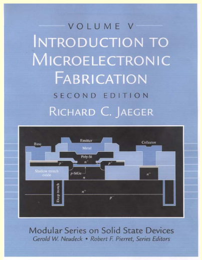
# Thermal Oxidation Example
## Mathematical Solution




(b) From Table 3.1,

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

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

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

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



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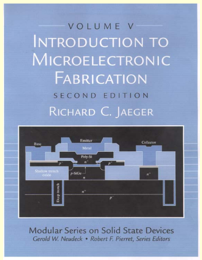
# Thermal Oxidation
# Wet High Pressure Oxidation



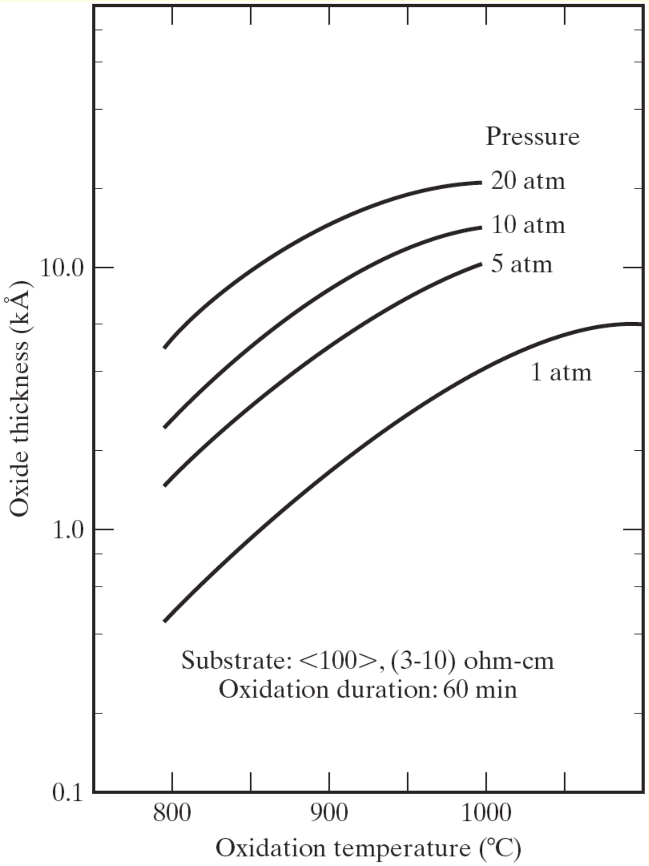
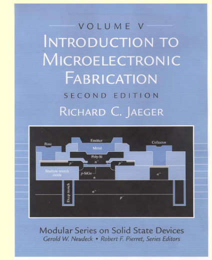




FIGURE 3.8

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



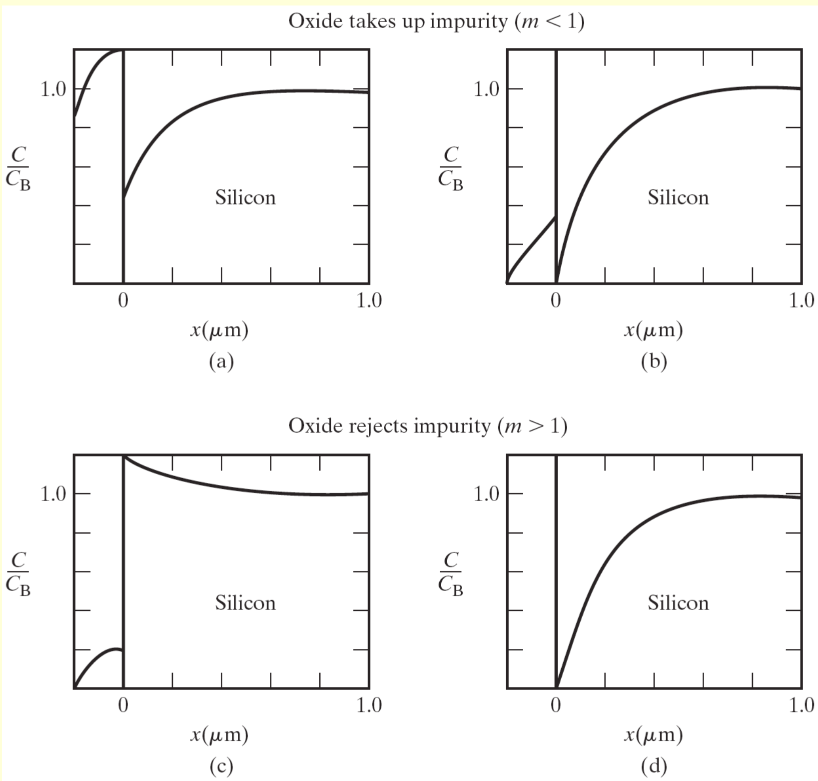




FIGURE 3.9

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].



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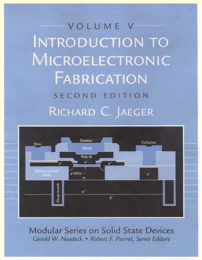
# Thermal Oxidation Masking Properties of $SiO_2$



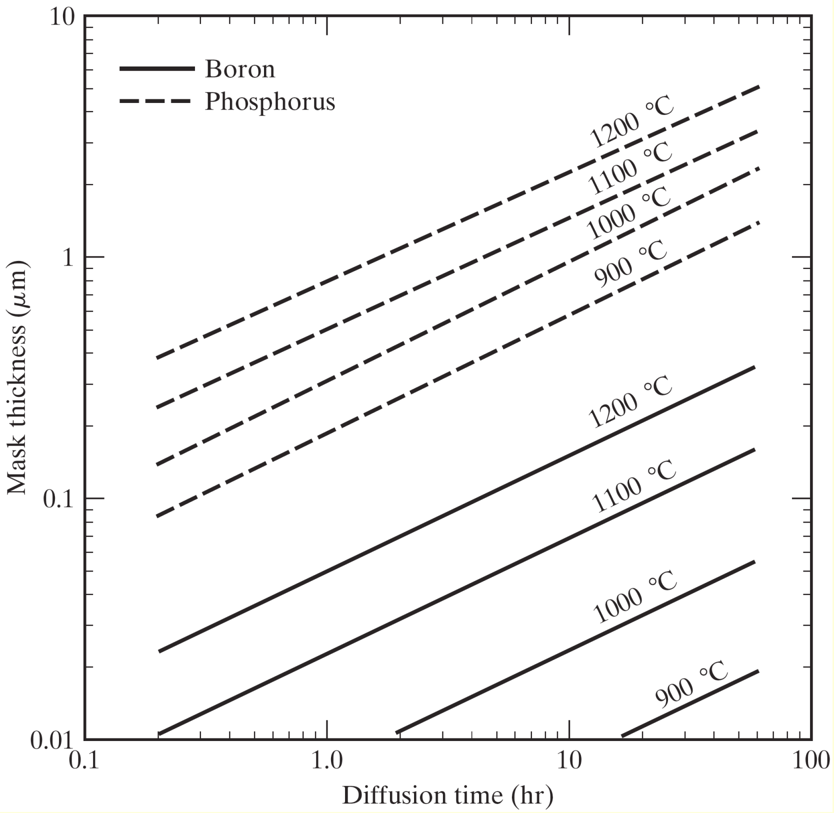
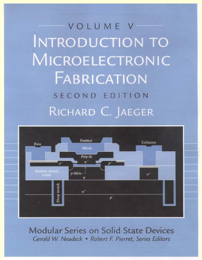




FIGURE 3.10

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



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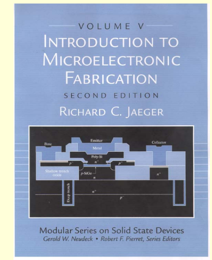
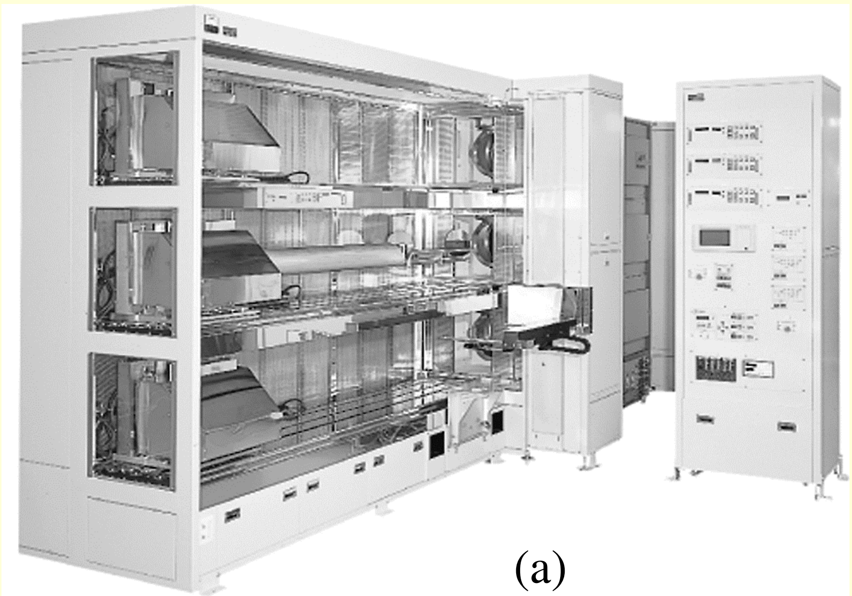
# Thermal Oxidation
# Oxidation Systems



(a)

(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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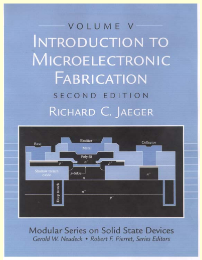
# Local Oxidation of Silicon (LOCOS)



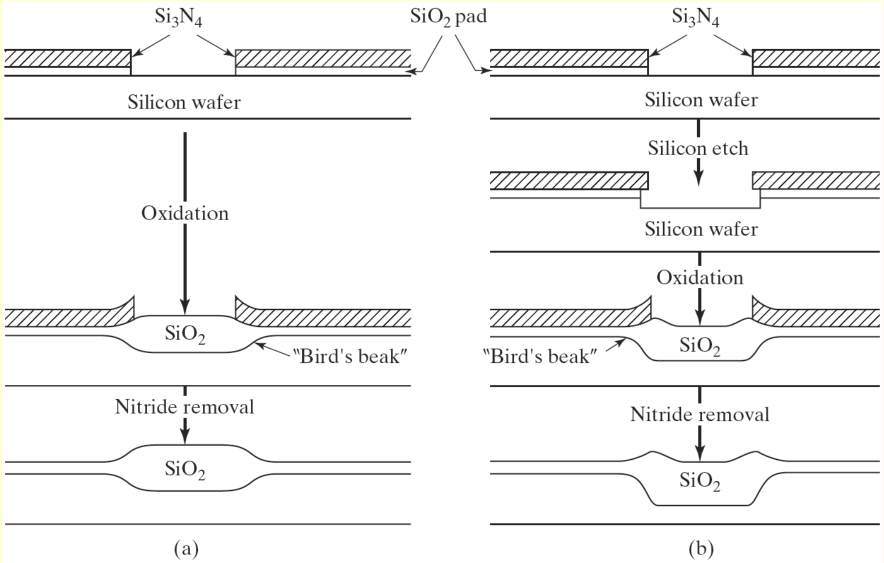
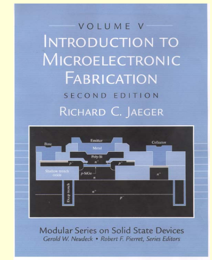




FIGURE 3.12

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

# Thermal Oxidation
# Deep Trench Isolation



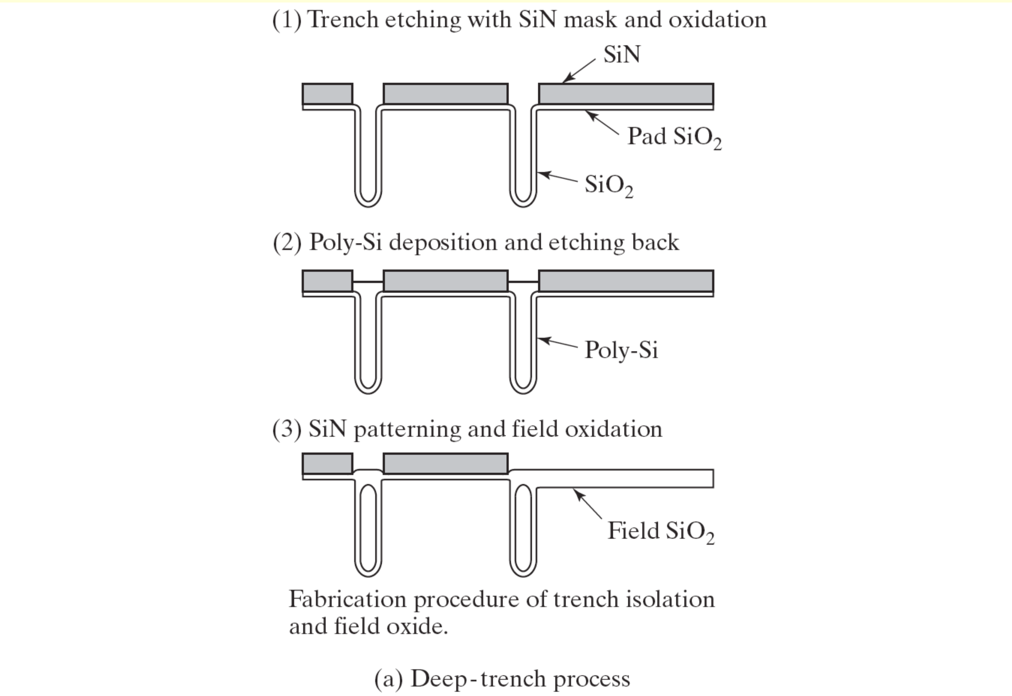
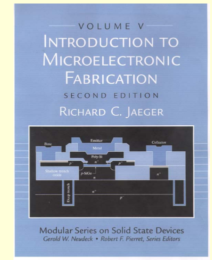



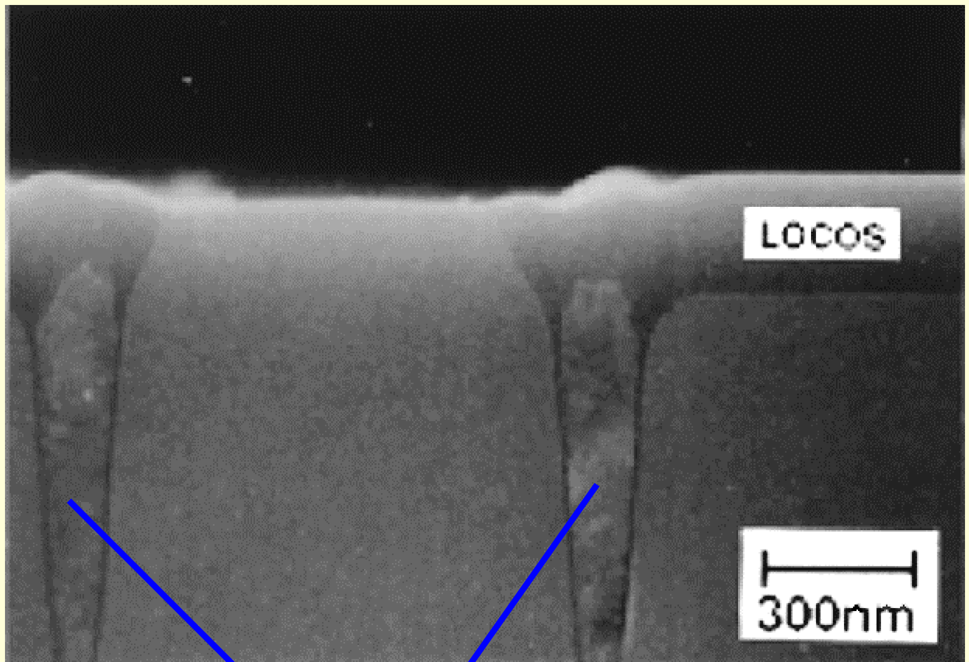

FIGURE 3.13

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].

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

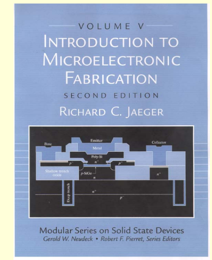
# Thermal Oxidation
## Example of Deep Trenches

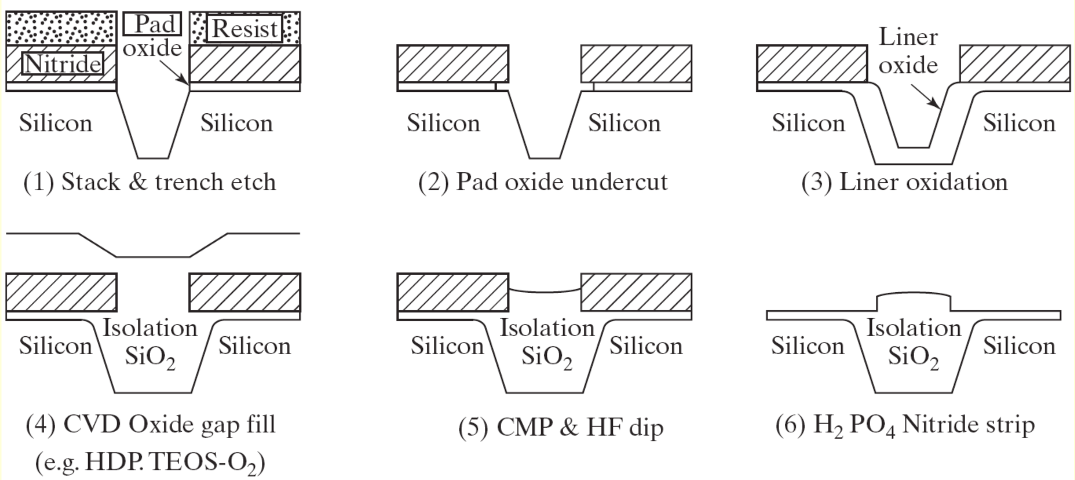



Filled Trenches

# Thermal Oxidation
# Shallow Trench Isolation



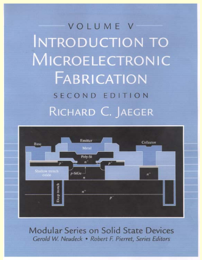

(b) Steps in a typical STI process flow

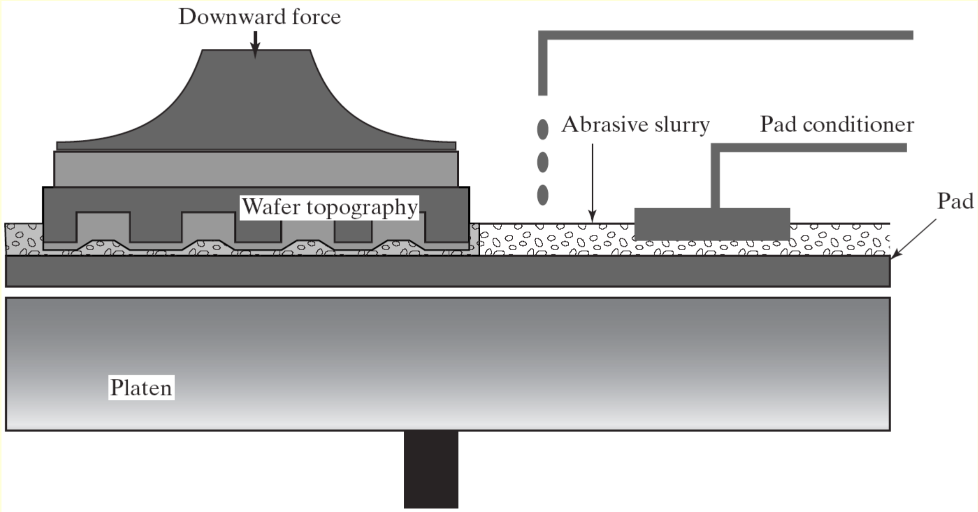
FIGURE 3.13

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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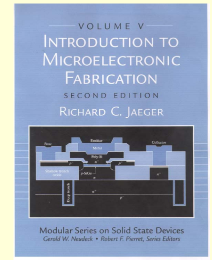
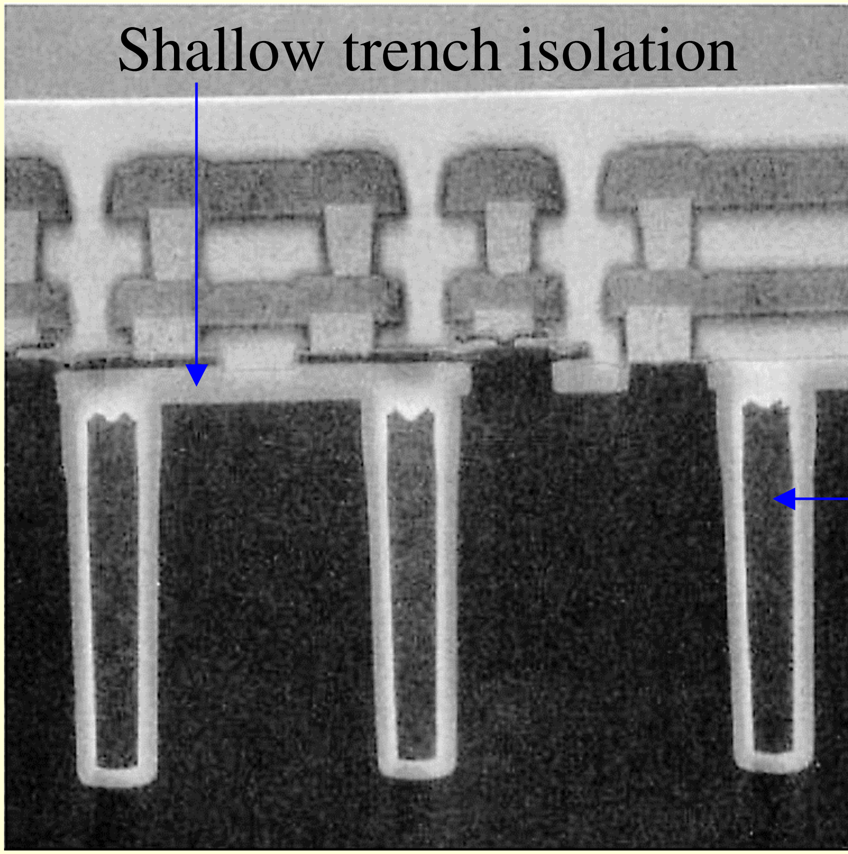
# Thermal Oxidation Trench Isolation Example




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].



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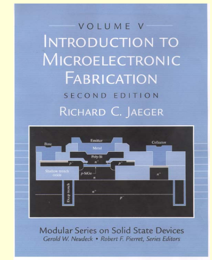
# Multilevel Metallization Using CMP



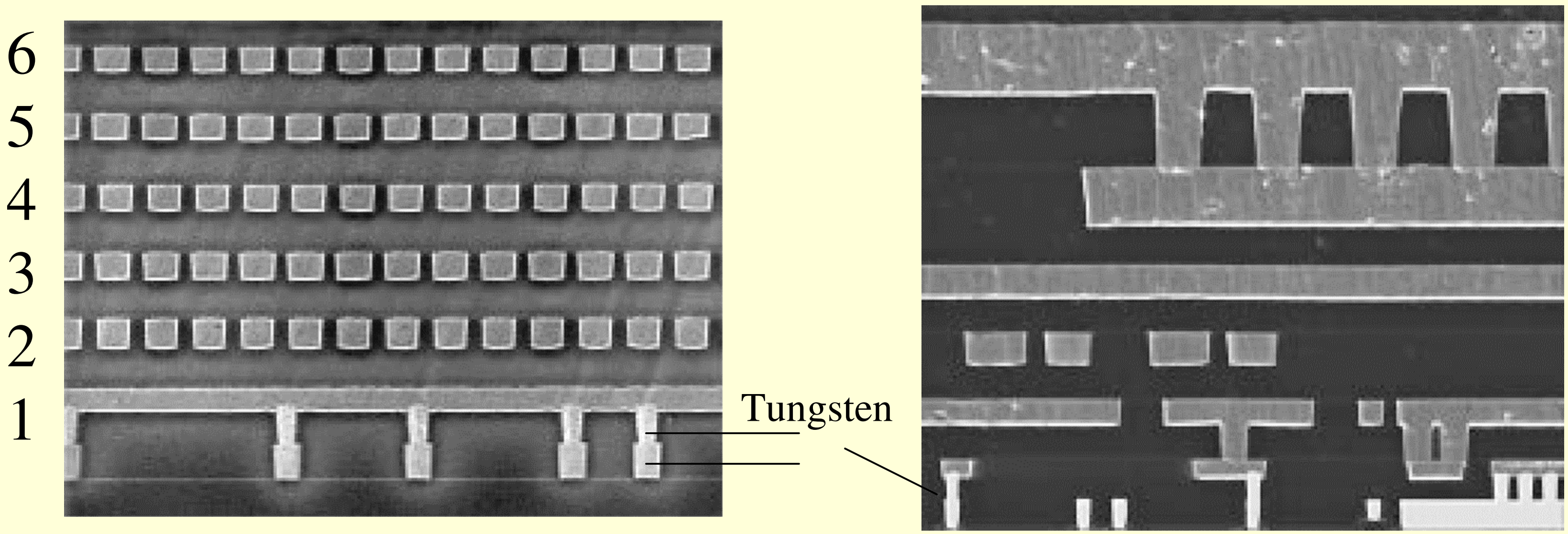




Figure 3.16 Multilevel metallization fabricated with chemical mechanical polishing (a) SEM of 6-level thin-wire copper. First-level copper is connected with tungsten studs to tungsten local interconnect. (b) SEM of 6-level copper with low RC metallization on levels 5 and 6. Copyright 1997 IEEE. Reprinted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

# Oxide Thickness Determination

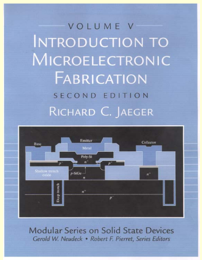



TABLE 3.2 Color Chart for Thermally Grown $SiO_2$ Films Observed Perpendicularly Under Daylight Fluorescent Lighting. Copyright 1964 by International Business Machines Corporation; reprinted with permission from Ref. [11].

| 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 | | |
| 0.17 | Metallic to very light yellow green | | |
| 0.20 | Light gold or yellow; slightly metallic | 0.72 | Blue green to green (quite broad) |
| | | 0.77 | "Yellowish" |
| 0.22 | Gold with slight yellow orange | 0.80 | Orange (rather broad for 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 $SiO_2$)

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

- Ellipsometer - direct measurement



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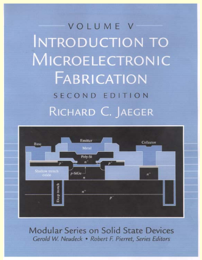
# Process Simulation

## SUPREM Oxidation Example



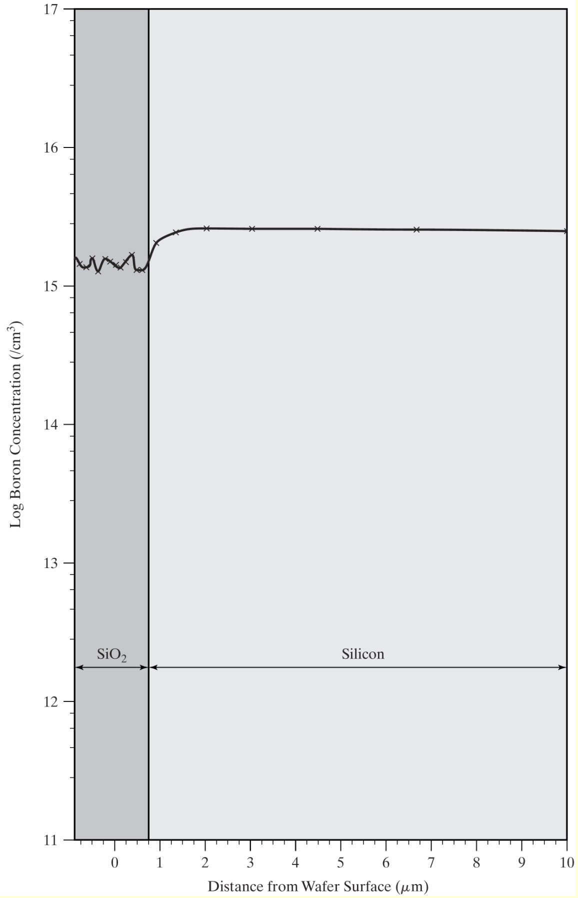




FIGURE 3.17

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

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

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.02 = 5
DIFFUSION TEMP=1100 TIME=60 T.FINAL = 800 F.N2 = 5
$ Print layer information
....
....
$ Plot results
....
....
```



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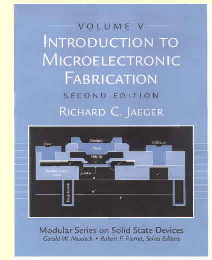
# Thermal Oxidation References

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# End of Chapter 3



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