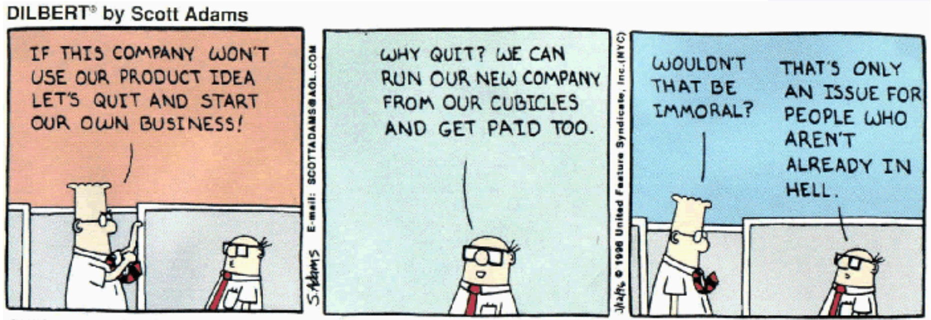
Fundamentals of Micromachining



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BIOEN 6421
EL EN 5221 and 6221
ME EN 5960 and 6960

Basic Materials Science for MEMS

- Basic material interactions
- Silicon as a material
- Crystallography
- Crystal defects and impurities
- Wafer manufacture
- Stress and strain
- Review of class projects

Sensors and Actuators

- “Sensor” (Latin sentire meaning “to perceive”)
- “Transducer” (Latin transducere meaning “to lead across”)
- A sensor performs a transducing action and the transducers must necessarily sense some physical or chemical signals
- Types of signals: chemical, electrical, magnetic, mechanical, radiant, thermal

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Materials Overview

- Metals
  - Characterized by metallic bonds
- Polymers
  - Long chain molecules of repeating units
- Ceramics
  - Inorganic compounds with ionic and covalent bonding
- Others- glass (non-crystalline solids) and carbon

Basic Atomic Interactions

- Ionic
  - Electrostatic bonding
- Covalent
  - Electron sharing
- Metallic
  - Electron fluid or gas
- Hydrogen
  - Ionic interactions between covalently bonded atoms
- Van Der Waals
  - Shifting interactions between atoms
- Crystals
  - Organized, repeating 3-D pattern of molecules or atoms
  - Closely packed structure

Material Properties

- Material failure
  - Yield stress
  - Ductile and brittle failure
  - Plastic deformation
  - Ultimate stress and strength
  - Some fail in shear, compression, tension
  - Fatigue- failure under cyclic conditions though well below yield stress
  - Creep- time dependent extension
    - Stress relaxation
  - Toughness
    - Energy absorption to failure
- Material properties
  - Consistent numbers not always available
  - Variation in runs, machines, locations
  - Structures generally a laminate composite
  - Properties may be function of fabrication process or post-processing
  - Measurement of key properties such as stress, Young's modulus, strength, and Poisson's ratio

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Surface Properties

- Surfaces are uniquely reactive
- Surfaces are different from the bulk
- Surfaces are readily contaminated
- Surface material/ structure is mobile
  - Can change depending on environment
- Surface structures or properties
  - Roughness
  - Chemistry or molecules
  - Inhomogenous surfaces
  - Crystalline or disordered
  - Hydrophobicity (wettability)
    - Contact angle

Surface Measurements

- Contact angle
- ESCA - Electron Spectroscopy for Chemical Analysis
  - Element identification and bonding state (XPS)
- Auger Electron Spectroscopy
- SIMS(Secondary Ion Mass Spectrometry)
  - Element ID, Low concentrations, Proteins
- FTIR- ATR (Fourier Transform Infra Red)
  - Chemistry and Structure Orientation
- STM- Scanning Tunneling Microscopy
- SEM (Scanning Electron Microscopy)
- AFM (Atomic Force Microscopy)

Why Silicon?

- Available technology (IC circuits)
- Inexpensive
- Compatible with existing semiconductor technology (easy integration)
- Suitable for hybrid structures

- Types: amorphous, polycrystalline, crystalline

Silicon Wafer Characteristics

- Orientation (cleavage or fracture)
- Si cleaves between (111) planes, III-V separate on (110)
- Roughness
- Flatness
- Orientation of primary and secondary flat
- Type n or p
- Surface misorientation
- Si resistance
- Thickness
- Backside damage is induced if required
- Rounded wafer edge (significantly reduces edge chipping, wafer breakage, photoresist build up)

Wafer Flats

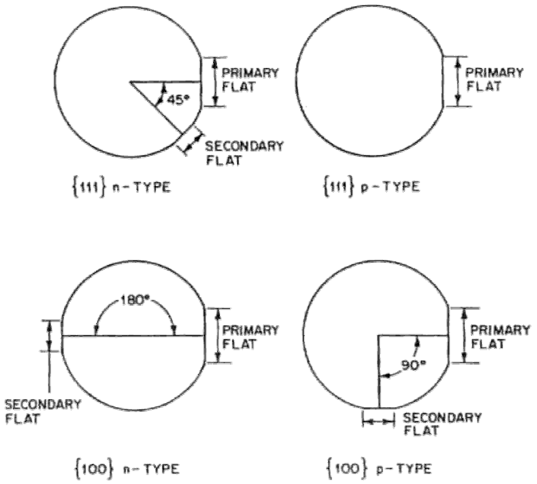


FIGURE 4.5 Primary and secondary flats on silicon wafers.

Stress and Strain

- Stresses are forces applied over areas
- Strain is a dimensional change due to an applied stress
- Axial stress and strain $\sigma = \frac{F}{A}$ $\varepsilon = \frac{\Delta L}{L_0}$
- Tension +, compression -
- Hooke's law- stress and strain proportional
- Young's modulus- $E = \frac{\sigma}{\varepsilon}$
- Shear stress and strain $\tau = \frac{F}{A}$ $G = \frac{\tau}{\gamma}$
- Shear modulus- G, γ is an angle
- Poisson's ratio- lateral distension for axial load

$$\nu = \frac{transverse}{longitudinal} = -\frac{\varepsilon_t}{\varepsilon_a}$$

Stress and Strain Relationships

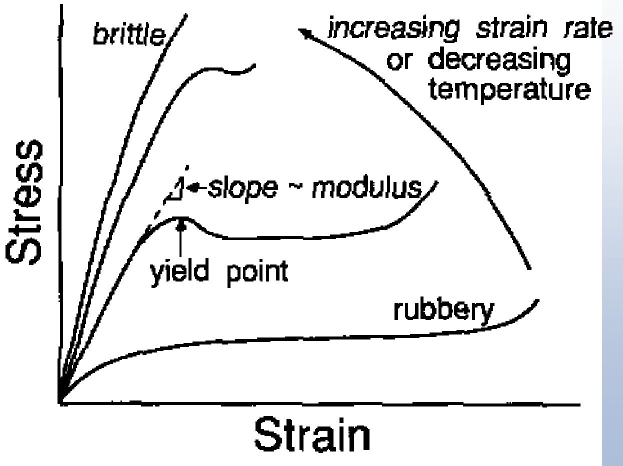


FIG. 6. Tensile properties of polymers.

Miller Indices in Crystals

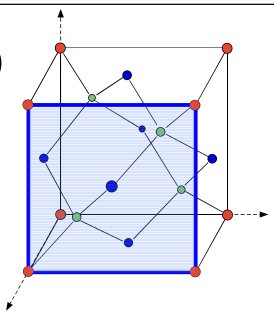
- For a plane with:
  - x-axis intercept x_o
  - y-axis intercept y_o
  - z-axis intercept z_o
  - the Miller indices (hkl) for this plane are given by finding the inverses of x_o, y_o, & z_o and reducing them to the smallest set of integers h: k: l having the same ratio $(x_o)^{-1}$: $(y_o)^{-1}$: $(z_o)^{-1}$.
- Conventions:
  - (hkl): single plane or set of all parallel planes.
  - $(\bar{h}\,kl)$: for a plane that intercepts the x axis on the negative side of the origin.
  - {hkl}: for all planes of equivalent symmetry, such as {100} for (100), (010), (001), $(\bar{1}00)$, $(0\bar{1}0)$, and $(00\bar{1})$ in cubic symmetry.
  - [hkl]: for the direction perpendicular to the (hkl) plane.
  - <hkl>: for a full set of equivalent directions.

Silicon as a mechanical material for MEMS fabrication

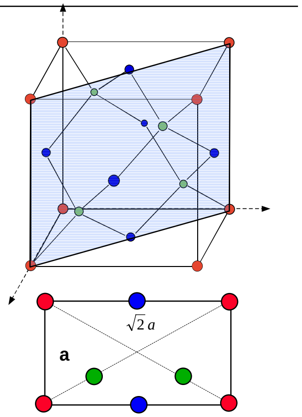
- classic reference in the field:
  - K.E. Petersen "Silicon as a Mechanical Material", *Proceedings of the IEEE*, Vol. 70, No.5, May 1982.
    - http://robotics.eecs.berkeley.edu/~tahhan/MEMS/petersen/mems_petersen.htm
  - tenants:
    - silicon is abundant, inexpensive, and can be produced in extremely high purity and perfection;
    - silicon processing based on very thin deposited films which are highly amenable to miniaturization;
    - definition and reproduction of the devices, shapes, and patterns, are performed using photographic techniques that have already proved capable of high precision;
    - silicon microelectronic (and therefore also mems) devices are batch-fabricated.

Low Index Directions In Silicon (Cubic, Diamond Structure)

- (100)



- (110)



surface atomic density

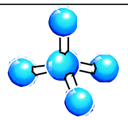
$$\rho_{100}^{surface} = \frac{\left(1atom + 4\cdot\left[\tfrac{1}{4}atom\right]\right)}{a^2}$$

silicon:

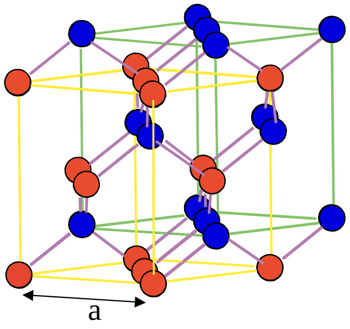
ρ_{100} = 6.8 x 10^{14} atoms / cm^2

$$\rho_{110}^{\text{surface}} = \frac{\left(2\,\text{atoms} + 4\cdot\left[\tfrac{1}{4}\,\text{atom}\right] + 2\cdot\left[\tfrac{1}{2}\,\text{atom}\right]\right)}{\sqrt{2}\,\text{a}\cdot\text{a}}$$

Silicon crystal structure

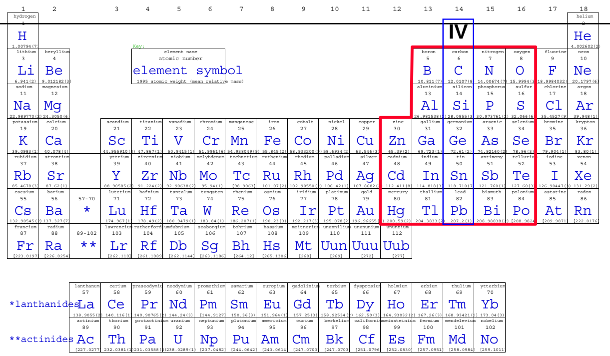


- valence 4 structure
  - each atom bonds to four neighbors in a tetragonal configuration
- crystal lattice is face centered cubic (FCC), with two atom basis [at (0,0,0) and (1/4, 1/4, 1/4)]: Zincblende
    - two "interpenetrating" FCC lattices
  - lattice constant "a": cube side length
    - silicon (rm temp): 5.43 Å
    - nearest neighbor distance $d_n = \frac{\sqrt{3}}{4}a$
  - atomic density:
    - 4 atoms inside cube
    - 6 atoms "half" inside at face centers
    - 8 atoms 1/8 inside at corners
    - total of 8 atoms per cube: atomic density 8 / a^3



ρ_{Si} = 5×10^{22} atoms/cm^3

Dopants and impurities in semiconductors



- For column IV elements (e.g., silicon)
  - valence III: one electron “short”, acceptor
    - boron, aluminum, gallium
  - valence V: one “extra” electron, donor
    - nitrogen, phosphorus, arsenic, antimony

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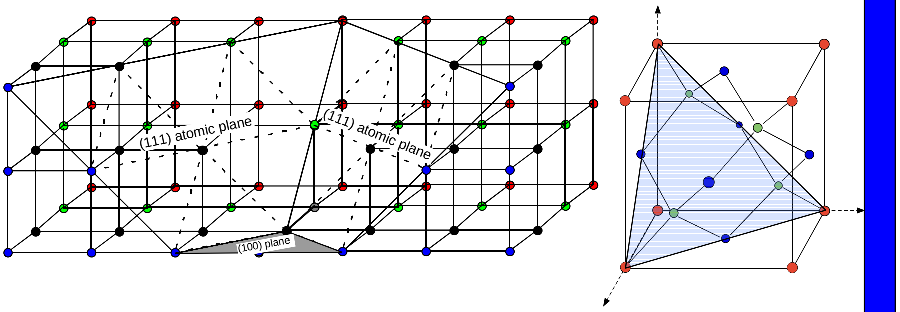
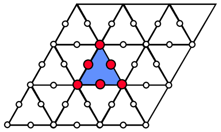
(111) planes

- (111) planes etch the slowest, tend to be cleavage planes



$$\rho_{111}^{surface} = \frac{\left(3\cdot\left[\frac{1}{2}\text{ atom}\right] + 3\cdot\left[\frac{1}{6}\text{ atom}\right]\right)}{\frac{\sqrt{3}}{2}\cdot a^2}$$



- silicon:
  7.8 x 10^{14} atoms / cm^2
- surface atomic density somewhat higher than (100)

Impurities in Silicon

- Oxygen: (column VI)
  - common unintentional impurity from silica crucibles
    - 10^{16} - 10^{18} cm^{-3}
    - usually clumps with silicon into large (~1μm) SiO_2 complexes; sensitive to processing history
- Carbon: (column IV)
  - high solid solubility ($4x10^{18}$)
  - mainly substitutional, electrically inactive
- Gold:
  - deep donor or acceptor
  - rapid diffuser
  - minority carrier lifetime "killer"

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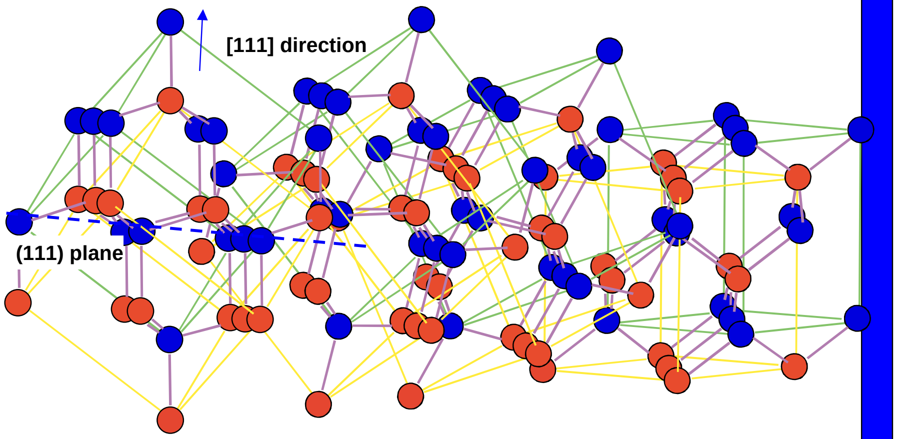
(111) orientation in silicon

- [111] is the “natural” orientation for zincblende crystals



Point Defects in Crystals

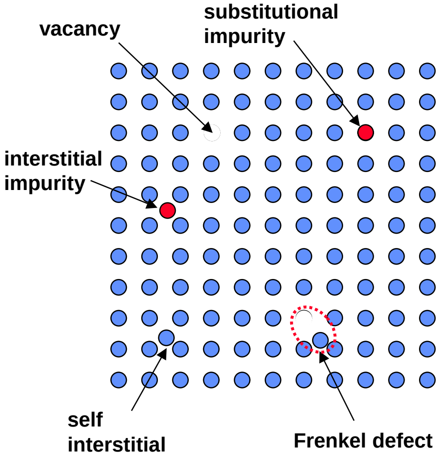
- vacancy , interstitial , substitutional
  - isolated vacancy: Schottky defect

    $$n \cong N_{\text{atomic}} e^{-E/kT}$$

    - $E_{\text{formation}}$ ~ 2 eV
      - T = 300K: n ~ 0
      - T = 1300K: n ~ 10^{13}
  - vacancy-interstitial pair: Frenkel defect

    $$n \cong N_{\text{atomic}} e^{-E/2kT}$$

    - $E_{\text{formation}}$ ~ 1 eV
      - T = 300K: n ~ 10^{13}
      - T = 1300K: n ~ 10^{20}



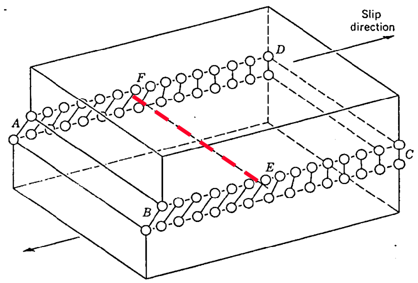
Solid solubility limits in Si

- solid solubility: maximum equilibrium concentration of impurity (solute) in host material (solvent)
  - temperature dependent
  - generally lower at lower temp
  - @ 1000˚C

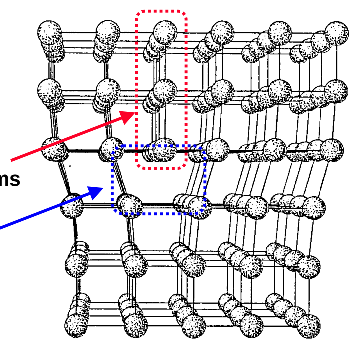
element
$N_{\text{solid sol}}$
(cm^{-3})

		B 1.5 x 10^{20}	C	N
		Al 2 x 10^{19}	Si	P 10^{21}
Cu	Zn	Ga 3 x 10^{19}	Ge	As 2 x 10^{21}
Ag	Cd	In	Sn	Sb 4 x 10^{19}
Au 10^{16}	Hg	Tl	Pb	Bi

Edge Dislocations



$\overline{EF}$ is dislocation line



from Kittel, p. 591

- one dimensional defect
  - formation energy is high, concentration usually low

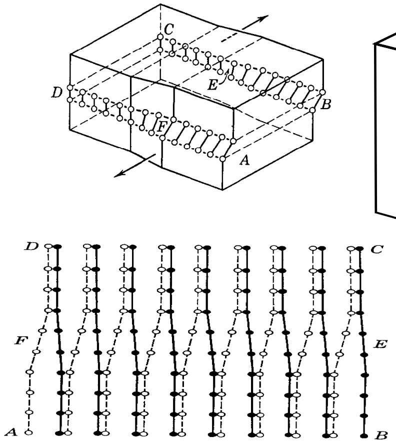
Defects in crystals

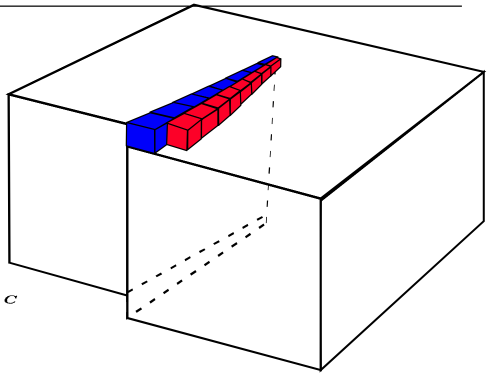
- point defects
  - "zero" dimensional
  - most common, lowest energy of formation
- dislocations or line defects
  - one dimensional
  - collection of continuous point defects
- area (planar) defects
  - two dimensional
  - gross change in crystal "orientation" across a surface

Bulk crystal growth

- melting points
  - silicon: 1420˚ C
  - quartz: 1732˚ C
- starting material: metallurgical-grade silicon
  - by mixing with carbon, SiO_2 reduced in arc furnace
    - T > 1780˚C:
      $SiC + SiO_2 \rightarrow Si + SiO + CO$
  - common impurities
    - Al: 1600 ppm (1 ppm = 5×10^{16} cm^{-3})
    - B: 40 ppm
    - Fe: 2000 ppm
    - P: 30 ppm
  - used mostly as an additive in steel

Screw Dislocation (1-d defect)





- screw dislocations are most commonly formed during crystal growth

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Preparation of electronic-grade silicon

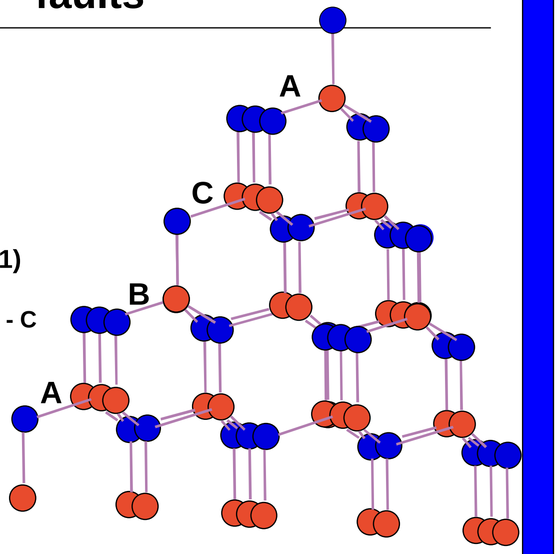
- gas phase purification used to produce high purity silicon
  - ~ 600˚C
  - crud + Si + HCl →
    - $SiCl_4$ (silicon tetrachloride)
    - $SiCl_3H$ (trichlorosilane)
    - $SiCl_2H_2$ (dichlorosilane)
    - chlorides of impurities
  - trichlorosilane (liquid at rm temp), further purification via fractional distillation
- now reverse reaction
  - $2SiHCl_3 + 2H_2 \text{ (heat)} \rightarrow 2Si + 6HCl$
  - after purification get
    - Al: below detection
    - B: < 1 ppb (1 ppb = 5×10^{13} cm^{-3})
    - Fe: 4 ppm
    - P: < 2 ppb
    - Sb: 1 ppb
    - Au: 0.1 ppb

Stacking arrangement and stacking faults

- layer ordering:

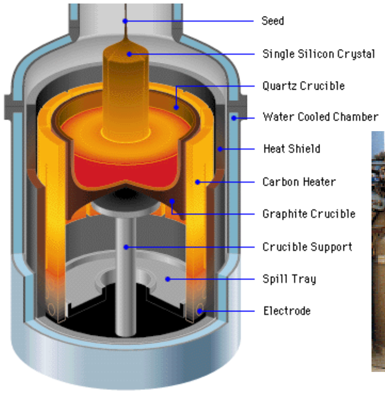
  A B C A B C

- planar (2-d) defect
  - stacking fault: missing or extra (111) plane
    - A - B - C - C - A - B - C
    - A - B - A - B - C

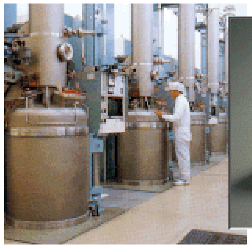


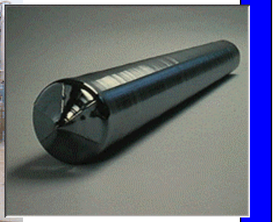
Czochralski crystal growth

- silicon expands upon freezing (just like water)
  - if solidify in a container will induce large stress
- CZ growth is “container-less”



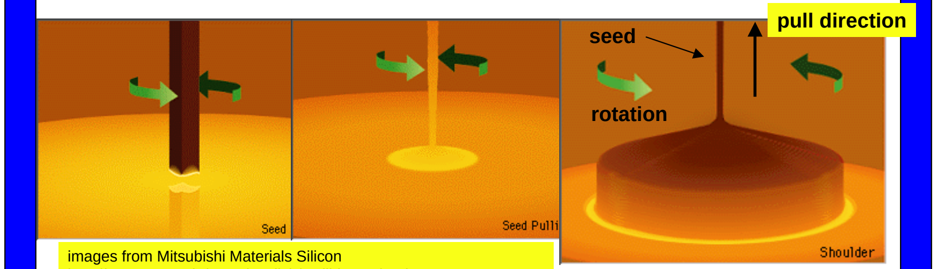
images from Mitsubishi Materials Silicon
http://www.egg.or.jp/MSIL/english/msilhist0-e.html





Diameter control during CZ growth

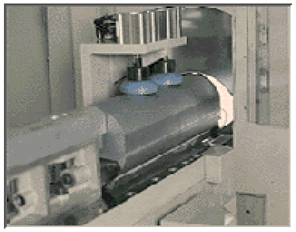
- critical factor is heat flow from liquid to solid
  - interface between liquid and solid is an isotherm
    - temperature fluctuations cause problems!
  - already grown crystal is the heat sink
    - balance latent heat of fusion, solidification rate, pull rate, diameter, temperature gradient, heat flow
    - diameter inversely proportional to pull rate (typically ~ mm/min)

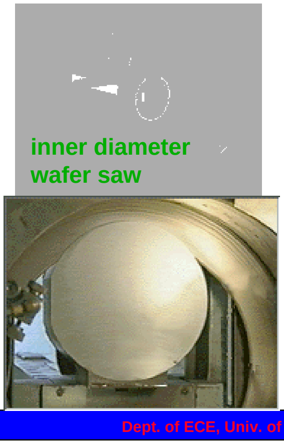


images from Mitsubishi Materials Silicon
http://www.egg.or.jp/MSIL/english/msilhist0-e.html

Wafer preparation

- boule forming, orientation measurement
  - old standard: “flat”perpendicular to <110> direction;
  - on large diameter “notch” used instead





- wafer slicing
  - <100> typically within ± 0.5˚
  - <111>, 2˚ - 5˚ off axis

images from Mitsubishi Materials Silicon
http://www.egg.or.jp/MSIL/english/msilhist0-e.html

Wafer prep (cont.)

- lapping
  - grind both sides, flatness ~2-3 µm
    - ~20 µm per side removed
- edge profiling
- etching
  - chemical etch to remove surface damaged layer
    - ~20 µm per side removed
- polishing
  - chemi-mechanical polish, SiO_2 / NaOH slurry
    - ~25 µm per polished side removed
  - gives wafers a “mirror” finish
- cleaning and inspection

Poisson's ratio

- **consider a bar under longitudinal tension or compression**
    - **under tension**
        - **length increases: Young's modulus**
        - **ALSO: cross sectional area decreases**
        - **this constitutes a transverse strain $\delta W/W$**
    - **Poisson's ratio ν = transverse strain / longitudinal strain**
        - **dimensionless (since both strains are dimensionless)**

$$\nu = \left(\frac{\delta W}{W}\right) \Big/ \left(\frac{\delta L}{L}\right)$$

$$\frac{\delta W}{W} = \frac{\nu}{E} \cdot (\text{longitudinal stress})$$

Wafer specifications

wafer diam.	thickness	thickness variation	bow	warp
150 mm ± 0.5mm	675μm ± 25μm	50μm	60μm	
200 mm ±				
300 mm ± 0.2mm	775μm ± 25μm	= 10μm		= 100μm

- **warp: distance between highest and lowest points relative to reference plane**
- **bow: concave or convex deformation**

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overall volume change

assume bar subjected to longitudinal tensile stress

$$V \propto (L+\delta L)\cdot(W-\delta W)^2 = (L+\delta L)\cdot\left(W^2 - 2W\cdot\delta W + \underbrace{[\delta W]^2}_{2\text{nd order} \approx 0}\right)$$

$$\approx (L+\delta L)\cdot\left(W^2 - 2W\cdot\delta W\right) = \underbrace{L\cdot W^2}_{\propto \text{ unstrained volume}} - 2W\cdot\delta W\cdot L + \delta L\cdot W^2 - 2W\cdot \underbrace{\delta W\cdot\delta L}_{2\text{nd order} \approx 0}$$

$$\approx \underbrace{L\cdot W^2}_{\propto \text{unstrained volume}} - 2W\cdot\delta W\cdot L + \delta L\cdot W^2 = L\cdot W^2 + W^2\cdot\delta L\cdot\left(1 - 2\cdot\frac{\delta W}{W}\cdot\frac{L}{\delta L}\right)$$

$$= L\cdot W^2 + \overbrace{W^2\cdot\delta L\cdot\underbrace{(1 - 2\cdot\nu)}_{\substack{<0 \text{ if } \nu > 0.5 \\ >0 \text{ if } \nu < 0.5}}}^{\text{volume change}}$$

- **ν > 0.5: total volume DECREASES under longitudinal tensile stress**
- **ν < 0.5: volume INCREASES**

Mechanical properties

- **consider elastic media: "Hooke's law" applies**
    - **restoring force is proportional to displacement**
- **consider a bar under longitudinal tension or compression**
    - **under tension**
        - **length increases**
        - **cross sectional area decreases**
        - **note TOTAL volume can increase or decrease, depending on material constants!**
- **relation between stress and strain**
    - **stress (longitudinal) = force per unit area (units of pressure!)**
    - **strain: fractional change in length $\delta L/L$ (dimensionless)**
    - **Young's modulus E = stress / strain (units of force per area)**
        - **i.e.,**

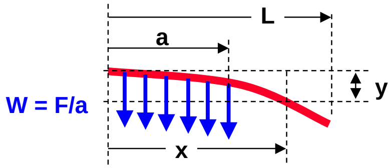
$$\text{stress} = E\cdot\frac{\delta L}{L}$$

Young's modulus is the stress you would have to apply to double the length of the bar (I.e., $\delta L = L$)

http://www.britannica.com/seo/y/youngs-modulus/

Bending of a simple cantilever beam

- for a uniformly distributed force
  - W = (total force) / a



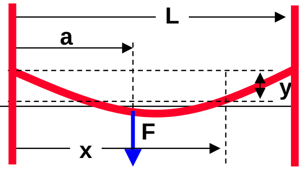
$$y(x) = \frac{W}{24 \cdot E \cdot I} \cdot \begin{cases} x^2 \cdot \left(6 \cdot a^2 - 4 \cdot a \cdot x + x^2\right) & x<a \\ a^3 \cdot \left(4 \cdot x - a\right) & x>a \end{cases}$$

Young's modulus and Poisson's ratio of "common" materials

- units
  - 10^6 pounds per square inch (psi) = mega-psi = 6.89×10^9 Newton/m^2 = 6.89 gigaPascal
- is temperature dependent

material	Young's modulus (@ 300K) (GigaPascal)	Poisson's ratio
diamond	1000	0.067
silicon	200	0.21
SiO2	70	0.17
Al2O3 (sapphire)	500	0.23
Iron	200	
Aluminum	70	0.34

Beam fixed both ends



- for beam fixed at both ends, point load

y_x is the vertical deflection of the beam

if x < a, $y_x = -(3 M_{x=0} x^2 + R_{x=0} x^3) / (6 E I_z)$

if x >= a, $y_x = -(3 M_{x=0} x^2 + R_{x=0} x^3 - W (x - a)^3) / (6 E I_z)$

$M_{x=0}$ is the bending moment reaction at the left hand support
$M_{x=0} = - F a (L - a)^2 / L^2$

$R_{x=0}$ is the vertical reaction force at the left hand end support
$R_{x=0} = F (L - a)^2 (L + 2 a) / L^3$

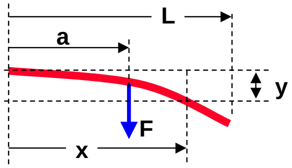
at load $y_{x=a} = -(3 M_{x=0} a^2 + R_{x=0} a^3) / (6 E I_z)$

y_{max} is the maximum deflection of the beam :
if a < L / 2, $y_{max} = 2 F a^2 (L - a)^3 / ((3 L - 2 a)^2 (3 E I_z))$
if a >= L / 2, $y_{max} = 2 F a^3 (L - a)^2 / ((L + 2 a)^2 (3 E I_z))$

x_{ymax} is the horizontal location maximum vertical deflection
if a < L / 2, $x_{ymax} = L - 2 L (L - a) / (3 L - 2 a)$
if a >= L / 2, $x_{ymax} = 2 L a / (L + 2 a)$

Static beam equations

- simple beam L long, w wide, t thick
  - beam: L >> w and t
- cantilever beam: supported at one end only
  - point force F at position a
  - displacement y at position x



$$y(x) = \frac{F}{6 \cdot E \cdot I} \cdot \begin{cases} x^2 \cdot \left(3 \cdot a - x\right) & x<a \\ a^2 \cdot \left(3 \cdot x - a\right) & x>a \end{cases}$$

  - E is Young's modulus
  - I is bending moment of inertia
    - for a rectangular cross section I is

$$I = \frac{1}{12} \cdot w \cdot t^3$$

  - note maximum displacement is at position L

$$y_{end}^{max} = \frac{F}{6 \cdot E \cdot I} \cdot a^2 \cdot \left(3 \cdot L^2 - a\right)$$

  - note deflection decreases as cube of thickness

beam calculator at:
http://www.ecalcx.com/beamanalysis/beamcantpoint_in.asp
other calculators at: http://www.ecalcx.com/

Thin film on thick substrate

- if film is stressed (stress σ), overall curvature results
  - E: Young's modulus; ν: Poisson's ratio; t_{sub}: substrate thickness; t_{film}: film thickness; r: radius of curvature

$$\sigma \approx \frac{E}{1-\nu}\cdot\frac{(t_{sub})^2}{t_{film}}\cdot\frac{1}{6\cdot r}$$

[1] A. Sinha, H. Levinstein, and T. Smith, "Thermal Stresses and Cracking Resistance of Dielectric Films on Si Substrates," *Journal of Applied Physics*, vol. 49, pp. 2423-2426, 1978.
[2] G. Stoney, "The Tension of Metallic Films Deposited by Electrolysis," *Proceedings of the Royal Society*, vol. A82, pp. 172, 1909.

Beam fixed both ends

- for beam fixed at both ends, distributed uniform load to a

Deflection y_x is the vertical deflection of the beam at x:

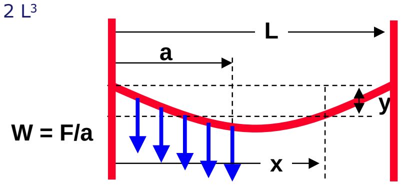
if x < a, $y_x = - (3 M_{x=0} x^2 + R_{x=0} x^3 - w x^4 / 4) / (6 E I_z)$

if x >= a, $y_x = - (3 M_{x=0} x^2 + R_{x=0} x^3 - w x^4 / 4 + w (x - a)^4 / 4) / (6 E I_z)$

$M_{x=0}$ is the bending moment reaction at left support:
$M_{x=0} = R_{x=L} L + M_{x=L} - w a^2 / 2$

$R_{x=0}$ is the vertical reaction force at the left support:
$R_{x=0} = w a - R_{x=L}$

$R_{x=L}$ is the vertical reaction force right support:
$R_{x=L} = w a^3 (2 L - a) / 2 L^3$



Dynamic response

- response of generic structure is approximately

$$\underbrace{m\frac{d^2x}{dt^2}}_{\substack{\text{mass*accel}\\ \text{NSL}}} + \underbrace{b\frac{dx}{dt}}_{\substack{\text{force}\propto\text{velocity}\\ \text{viscous damping}}} + \underbrace{k\cdot x}_{\substack{\text{elastic force}\\ \text{Hooke's law}}} = F_{\text{external}}$$

  - transfer function (Laplace domain)

$$H(s) = \frac{{}^{1}\!/_{m}}{s^2 + \left(\frac{b}{m}\right)\cdot s + \frac{k}{m}}$$

  - this is the same as an LRC circuit

$$H(s) = \frac{{}^{1}\!/_{LC}}{s^2 + \left(\frac{1}{RC}\right)\cdot s + \frac{1}{LC}} = \frac{\omega_o^{\,2}}{s^2 + \left(\frac{\omega_o}{Q}\right)\cdot s + \omega_o^{\,2}}$$

Deflection of a circular diaphragm

- much thinner than radius r
- for pinned around circumference, uniform force per unit area (i.e., uniform pressure P), no built in stress

$$\delta_{center} = \frac{3\cdot P\cdot r^4\cdot(1-\nu^2)}{16\cdot E\cdot t^3}$$