ELEC 315:
2 - Crystal structure and growth

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Outline

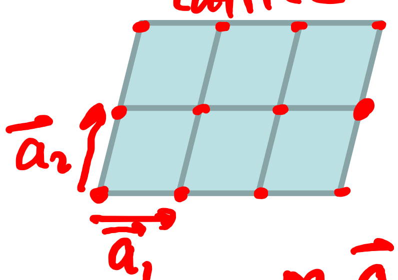
- Crystal structure in solids
- Crystalline, polycrystalline, amorphous materials
- Crystal growth
- Conductivity: Metals, semiconductors, and dielectrics

Crystal Structure

quartz

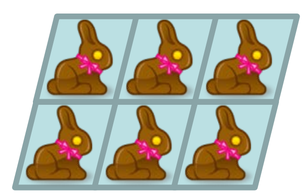
- Solid materials with ordered and periodic structure are called crystals. Examples: diamond (C), NaCl, Si, Sugar, liquid crystal (LC)
- The crystal appears exactly the same at one point as it does at the other equivalent points, once we know the periodicity. Crystals have a high degree of symmetry.
- The reason behind this well-ordered crystalline structure is the bonds between atoms and molecules.
- Examples of the type of bonds:
  - Covalent bond: Si
  - Ionic bond: NaCl
- The grid for repeating pattern in a crystal is called *lattice* and what is repeated is called *unit cell*.

lattice



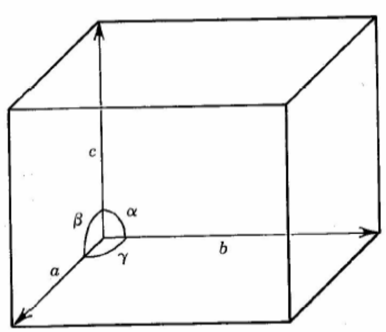
$m_1\vec{a}_1 + n_1\vec{a}_2$

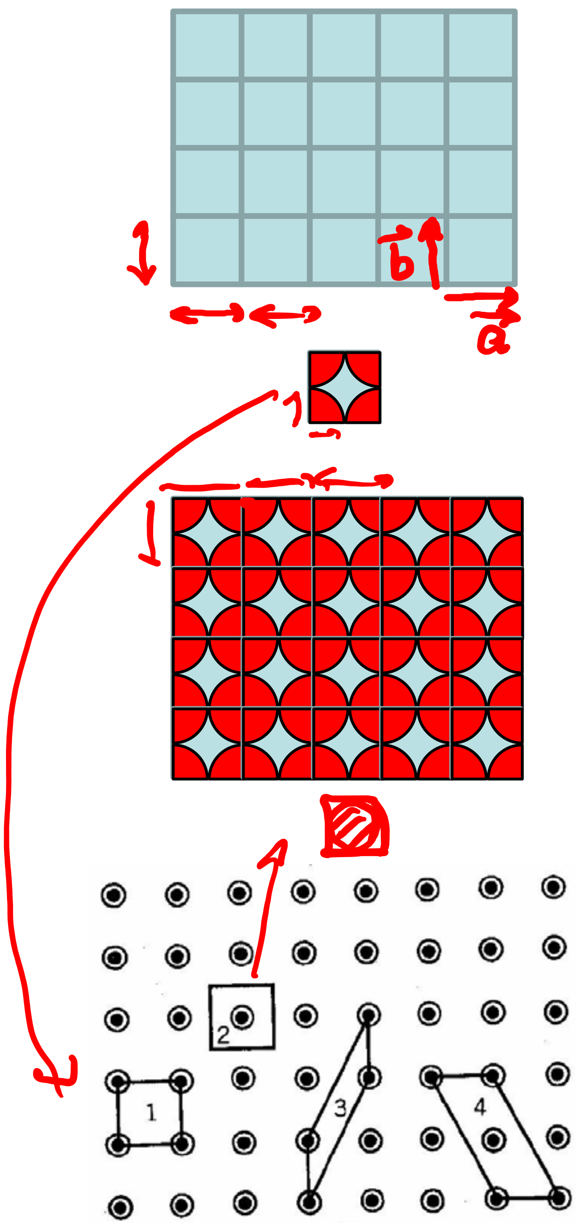
unit cell



Unit cell and basis vectors

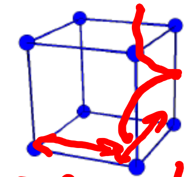
- A *unit cell* is a small volume that can be used to make the entire crystal when it is regularly repeated over the *lattice*.
- If we translate a unit cell by integral multiples of *basis vectors (lattice)* we reach another identical unit cell. The basis vectors link the unit cell to the lattice.
- A *primitive unit cell* is the smallest unit cell that can be used to form a specific crystal structure.





Different unit cells

- *Simple cubic (SC)* lattice: The unit cell is a cube and there is one atom at each corner of the unit cell. The side of the cube *a* is the period of the lattice.



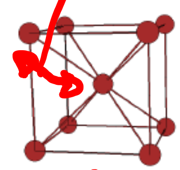
← a → lattice size

a = bond length = 2r

8 atoms × 1/8 (corner) = 1 atoms

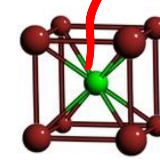
$$\frac{1 \text{ atom}}{a^3} \quad (cm^{-3})$$

- *Body-centred cubic (BCC)* lattice has an additional atom at the centre of the cube. (Na, Fe, Cr, …, CsCl, …)



bond length

← a →



Cs^+

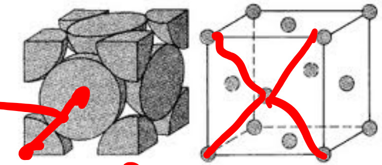
Cl^-

1 (centre) + 8 × 1/8 = 2 atoms

$$\text{bond length} = \frac{\sqrt{3}\,a}{2}$$

Different unit cells

- *Face-centred cubic (FCC)* lattice has atoms at the eight corners and centered on the six faces. (Cu, Al, Ni, Ag, …)



bL

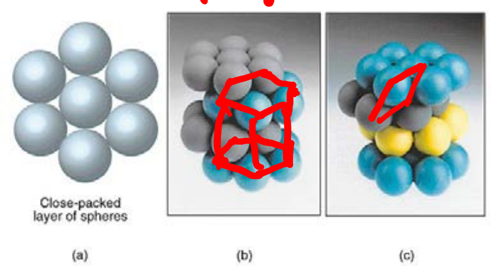
a

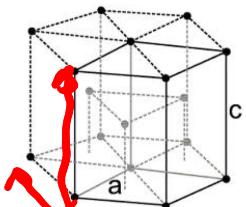
bond length $= \frac{\sqrt{2}}{2} a$

$$\underset{\text{corner}}{8 \times 1/8} + \underset{\text{face}}{6 \times 1/2} = 4 \text{ atoms}$$

- *Hexagonal closed-pack (HCP):* This structure provides closest layered packing for spheres. It is like (ABA in the figure) very similar to FCC (ABC in the figure).

HCP FCC



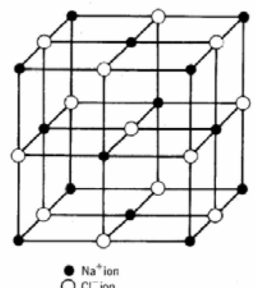


$$1/6 \times 12 + 2 \times 1/2 + 3 = 6 \text{ atoms}$$

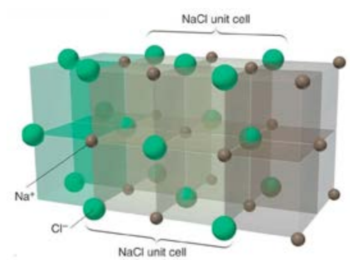
- NaCl crystal

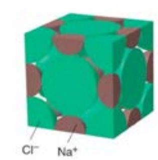
Na^+ : $8 \times 1/8 + 6 \times 1/2 = 4$ ions

Cl^- : $1 + 12 \times 1/4 = 4$ atoms



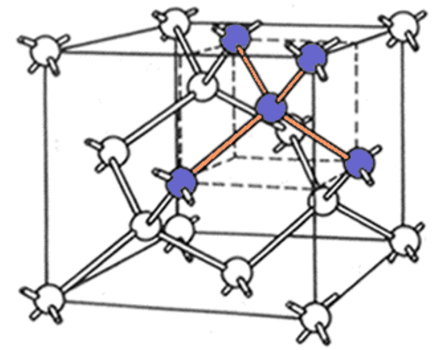
a



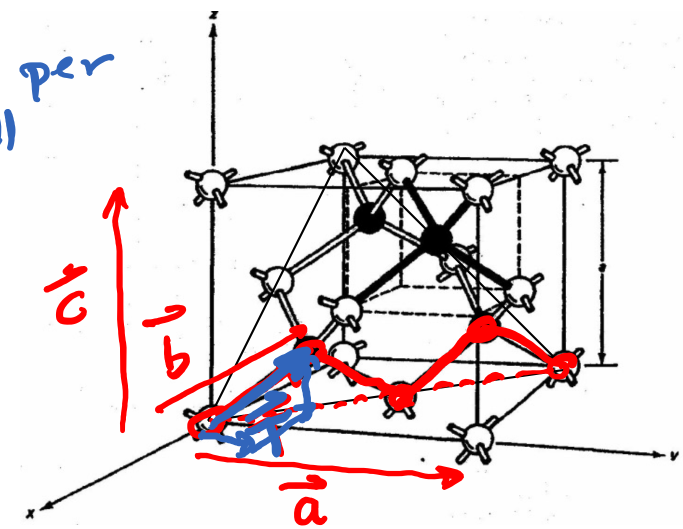


Crystal structure of Silicon

- *Diamond* unit cell: Semiconductors such as silicon and germanium have diamond lattice. In diamond lattice, each atom is symmetrically bonded to four other atoms in a tetrahedral configuration.
- The unit cell for a diamond lattice is made of a fcc unit cell with an extra atom placed at a/4+b/4+c/4 from each of the fcc atoms.



8 atoms per unit cell



$$\vec{T} = \frac{\vec{a}}{4} + \frac{\vec{b}}{4} + \frac{\vec{c}}{4}$$

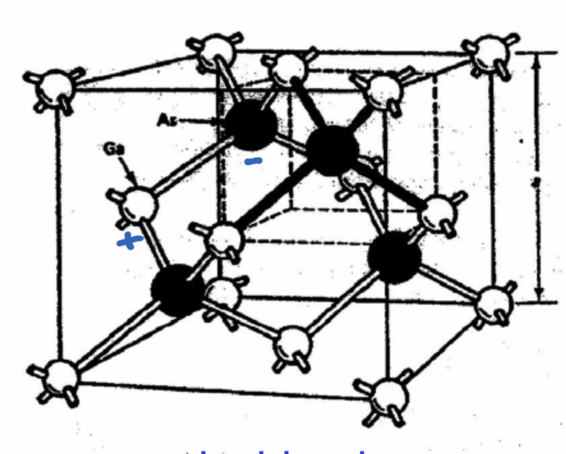
bond length $= |\vec{T}| = \frac{\sqrt{3}}{4} a$

See Pulfrey & Tarr 2.2

Zincblende Lattice

ZnS, ZnSe

- Many compound semiconductors (such as GaAs, InP, GaP, ZnS…) have a crystalline structure very similar to a diamond lattice, however, there are two types of atoms in the unit cell.
- These semiconductors have a *zincblende* lattice.



zincblende

GaAs stoichemtry

III-V semiconductor

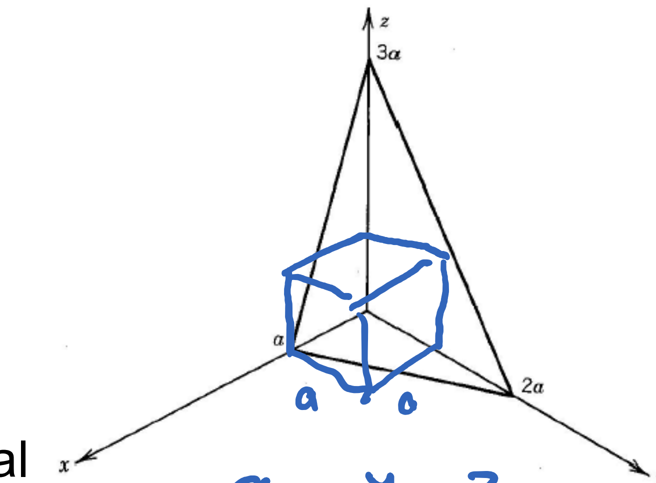
II-VI semiconductor

4 Ga atoms
4 As atoms

See Pulfrey & Tarr 2.2

Crystal planes

- To be able to refer to different crystal planes and directions in the crystal we use *Miller indices*.
- Three integers *(h k l)* is used to describe a plane in a crystal.
- To find these indices:
  - Find the intercept of the planes with the crystal axes as integral multiples of basis vectors.
  - Take the reciprocal of the integers and reduce them to smallest set of integers.
  - If intercept is negative, the integer is shown with a bar.



	x	y	z
intercepts →	a	2a	3a

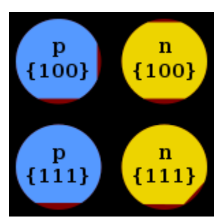
$\times 1/a$

1 2 3

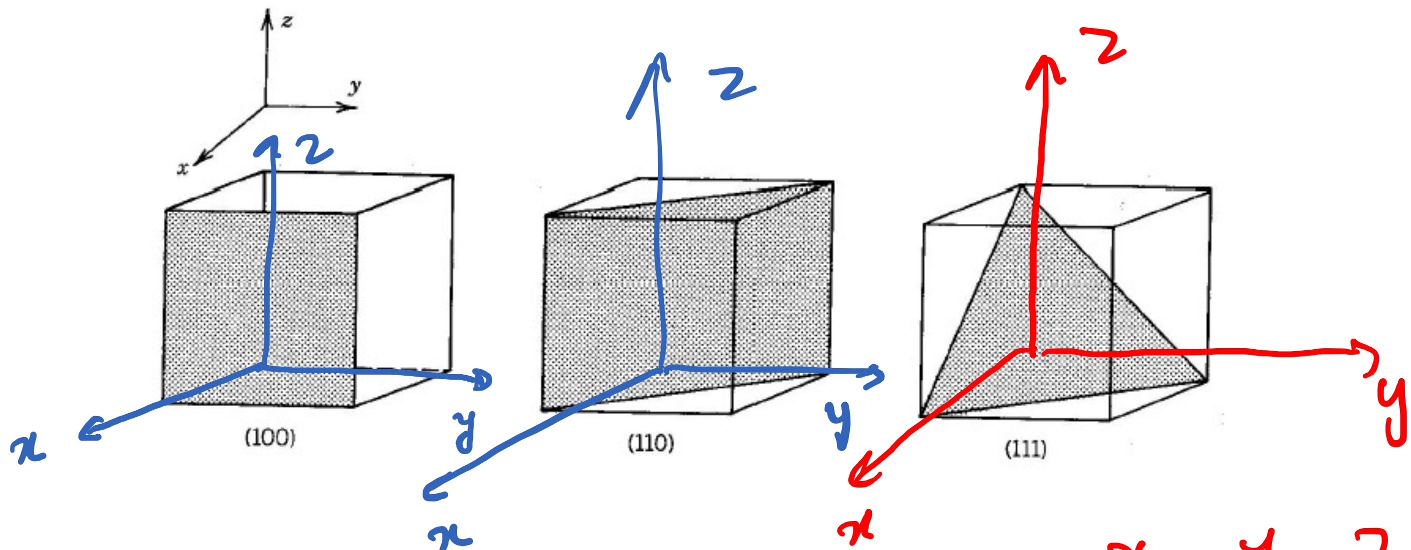
inverse

1 ½ 1/3

(632)



Example



x	y	z
a	∞	∞
1	∞	∞
1	0	0

(100)

x	y	z
a	a	∞
1	1	∞
1	1	0

(110)

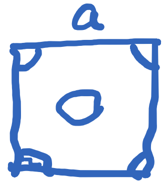
x	y	z
a	a	a
1	1	1

(111)

surface density

$2/a^2$

a



(100)

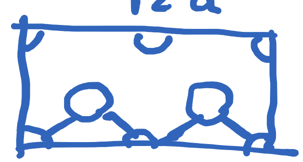
face planes

(010)

(001)

$\sqrt{2}\,a$

a



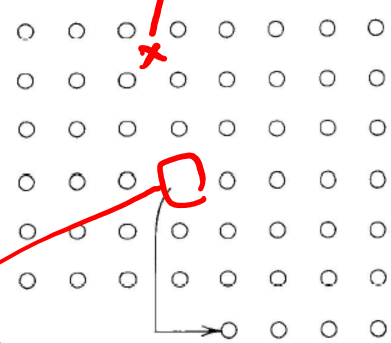
Crystal defects

$N_{Si} = 5 \times 10^{22}\ cm^{-3}$

$N_{defects} \sim 10^{10}\ cm^{-3}$

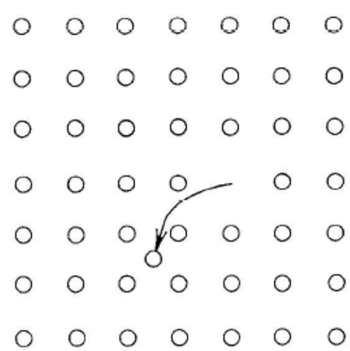
- In reality, the crystals are not perfect and contain a lot of defects. Examples of these defects:

interstitial

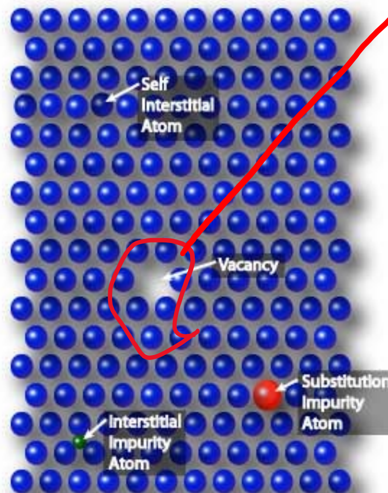


vacancy

doping

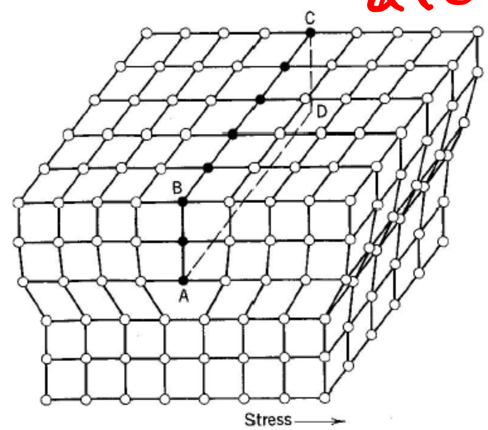


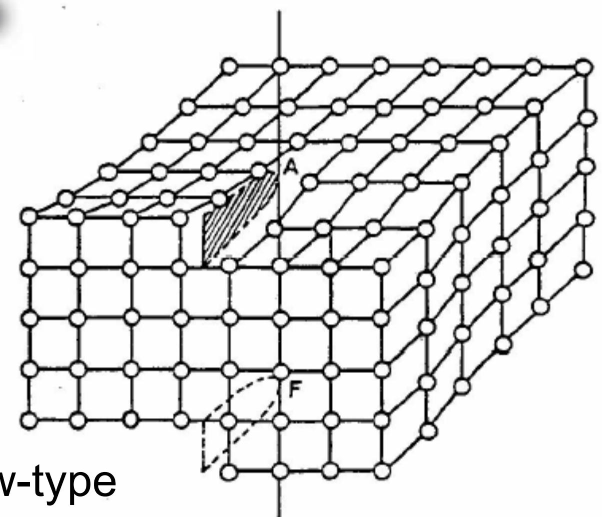
Point defects
(vacancy, interstitial)



dislocation

dopants
alloying





Screw-type
dislocation

Crystallinity

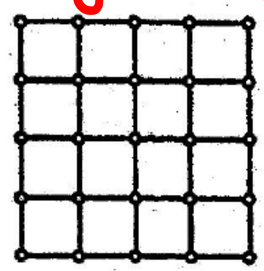
conductivity, mobility

$\sigma = q\,\mu_n\, n$

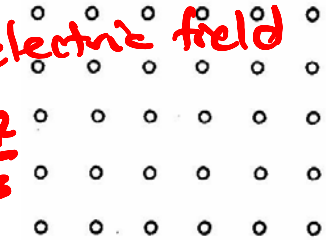
electron charge, electron density

- The crystalline structure of a solid determines its properties.
- Crystalline

mobility $\mu = \frac{v_d}{\mathcal{E}}$ drift velocity, electric field

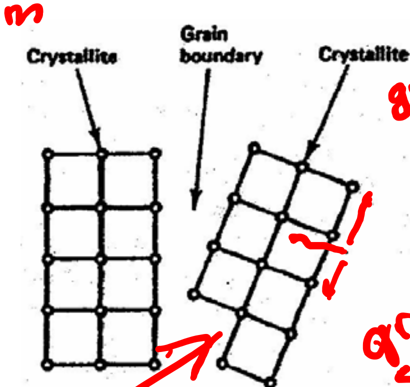


$\mu_n = 1350\ \frac{cm^2}{Vs}$



1μm – 1mm

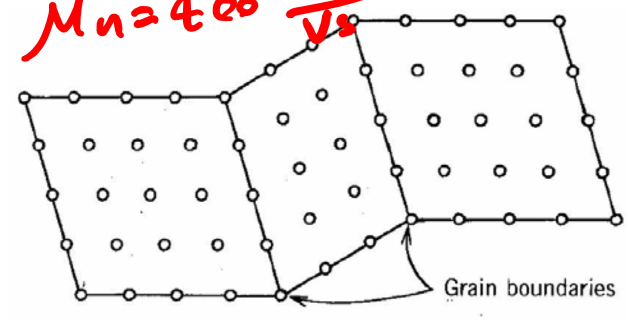
- Polycrystalline
- (microcrystalline)
- (nanocrystalline)



grains

grain size

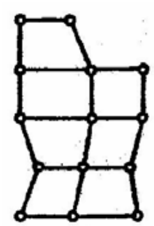
$\mu_n = 400\ \frac{cm^2}{Vs}$



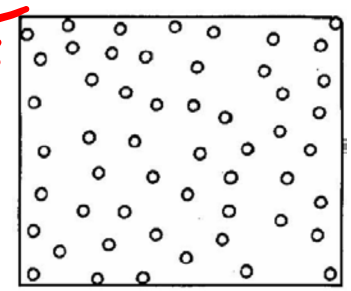
- Amorphous

disordered

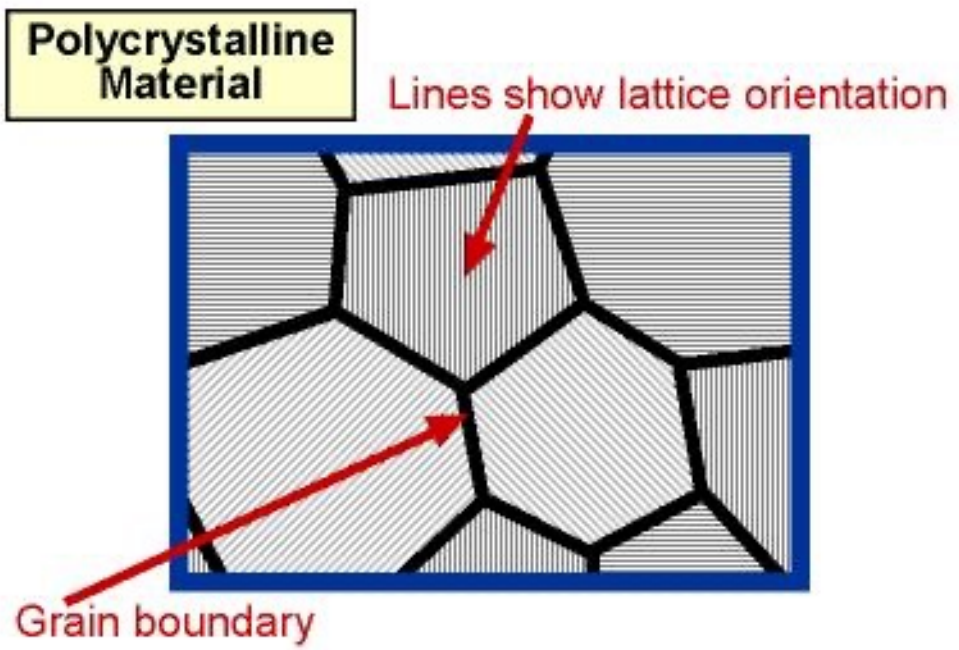
glass



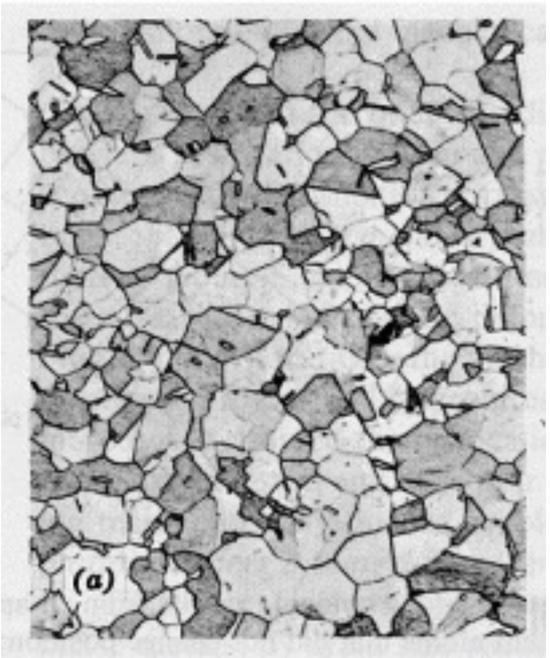
$\mu_n = 1\ \frac{cm^2}{Vs}$



Polycrystalline Materials



http://www.eng.auburn.edu/~wfgale/intro_metals/graphics/fig8_polycrys.jpg



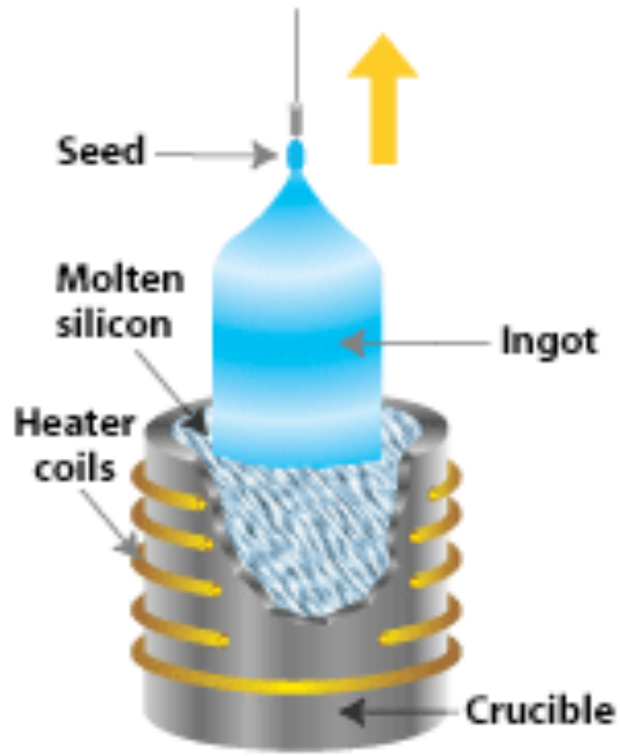
http://www.jwave.vt.edu/crcd/farkas/lectures/dislocations/fig9.gif

Amorphous

Single Crystal Growth

http://www.shef.ac.uk/~ch1mlt/teaching/chm337/si-crystal.jpg

Silicon Single Crystal
Up to 300 mm diameter



http://www.eere.energy.gov/solar/images/illust_czoch.gif

See Pulfrey & Tarr 2.2.2

Conductivity and Resistivity

- Conductivity and resistivity are important parameters that can be measured and define the type of the material.
- $\sigma = 1/\rho$ ($\Omega^{-1}cm^{-1}$ or S/cm)

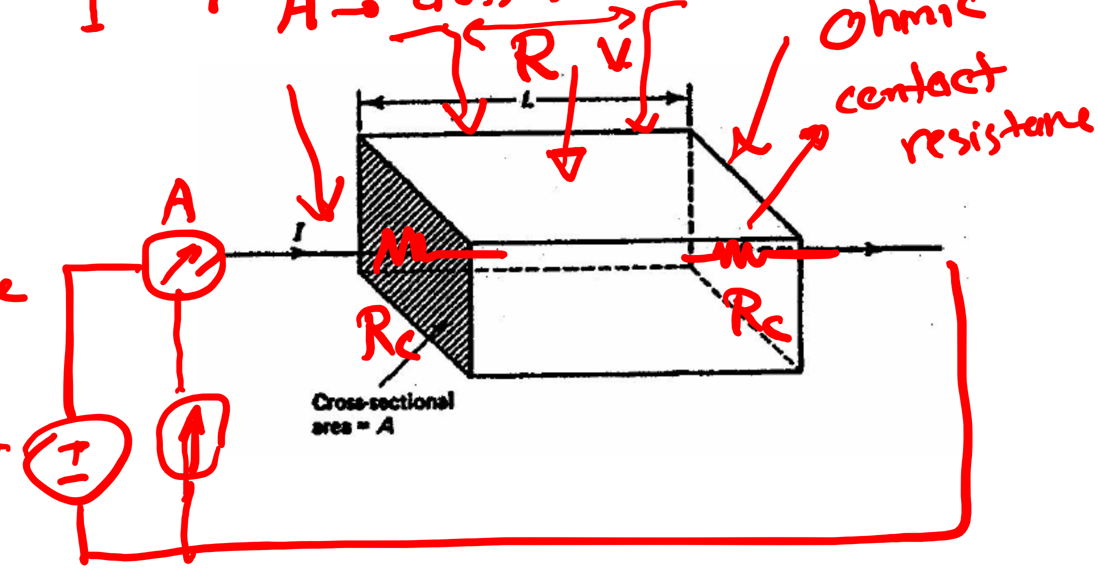
$\sigma = q \mu_n n$

10^{-8}	10^{-4}	1	10^{4}	10^{8}	10^{12}	10^{16}	10^{20}

metals | semiconductors | insulators — ρ (Ω-cm)

resistance $R = \frac{V}{I} = \rho \frac{L}{A}$ — L → length, A → cross section

$$\sigma = \frac{LI}{AV} = \frac{L}{AR}$$

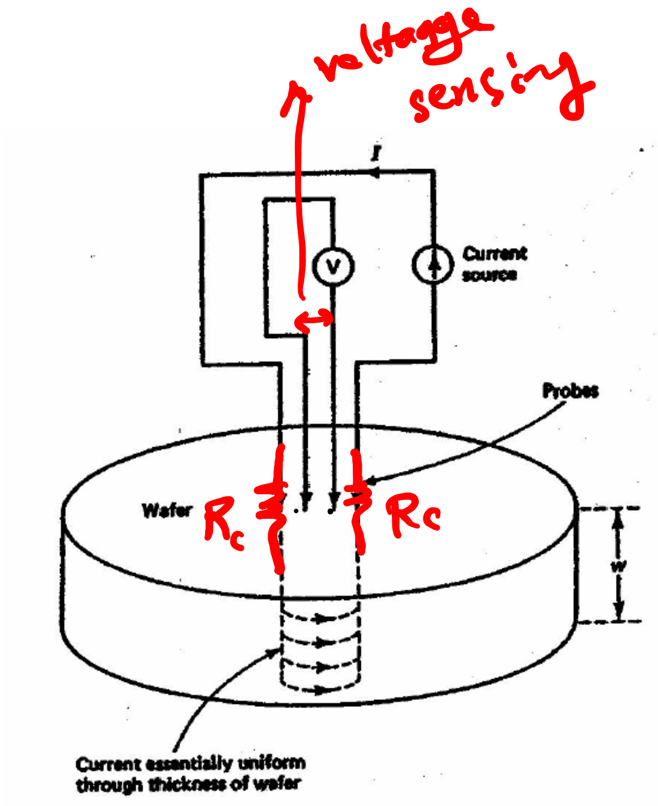


contact resistance

$R_M = R + 2R_c$

Four point probe

- To find conductivity of a (silicon) wafer, an important experiment is four point probe experiment.
- Four probes are used. A current I is passed through the outer probes and the voltage drop V over the inner probes are measured.
- For this experiment, the conductivity is give by



$$\sigma = \frac{I}{V}\frac{\ln 2}{\pi w}$$

width of wafer

Next lecture

- Basic quantum physics of semiconductors
- Reading for next week: Pulfrey and Tarr, Chapter 2: 2.1, 2.2
- Also read semiconductor quantum mechanics http://ece-www.colorado.edu/~bart/book/contents.htm 1.2.1-1.2.2 & 1.2.5-1.2.5.2.