Introductions June 5, 2023

The 3 Material Classes

① Metals (Fe, Cr, Cu, Zn, Al) → metallic bonds → band theory

② Ceramics (porcelain, concrete, advanced ceramics) → ionic bonds

③ Polymers ("plastics", Teflon®, Gore-Tex®, PP, PE, PMMA) → covalent bonds

- ceramics are brittle (they shatter)
  - ↳ often metal oxides

Exeptions

- wood, tissue (skin, carbon fiber, fibreglass
- composites
- semiconductors

Metals

- metallic element
- ductile (can be deformed permanently)
- shiny, and electrically and thermally conductive
- crystaline (highly organized at atomic level)

Ceramics

- hard, brittle
- non-conductive (electr. thermal)
- mostly metal oxides → ionic bonds
- crystaline or amorphous (disorganized)
- sappire (Al_2O_3), quartz (SiO_2), concrete

Introductions

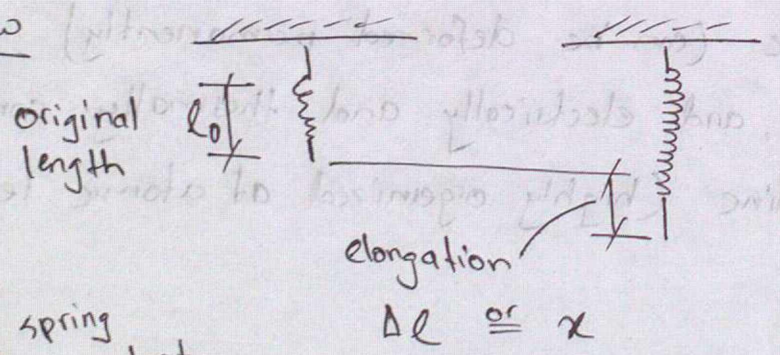
Polymers

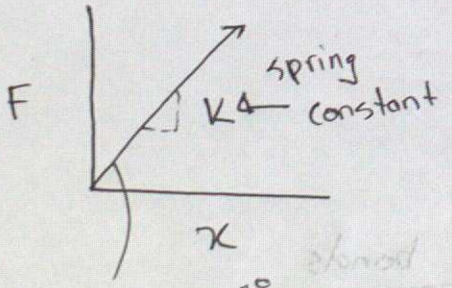
- ductile (not as stong as metals)
- non-conductive (electr. therm.)
- covalent bonds
- optically transluscent, opaque, or transperent
- polyethylene, PVC, epoxy, Styrofoam

Elastic Behaviour

- (Engineering) Stress and strain
- Young's Modules
- Strength
- Hooke's Law

Hooke's Law





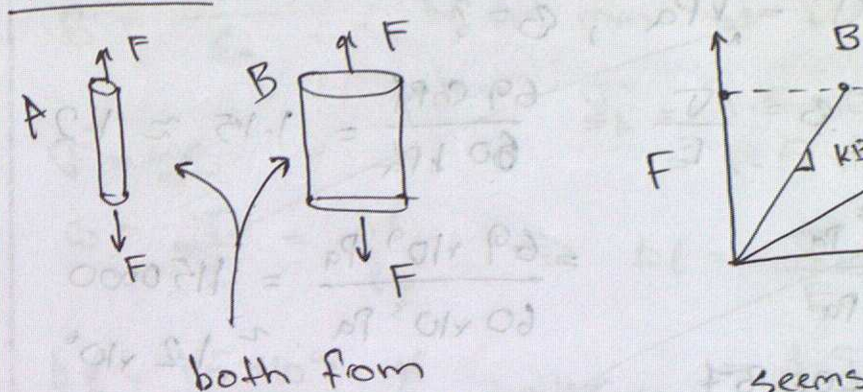
$y = mx + b \rightarrow 0$

$\boxed{F = kx}$ → Hooke's Law

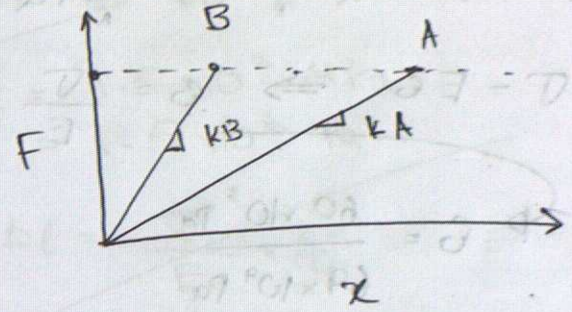
spring constant

Elastic Behaviour

Problem



both from same material



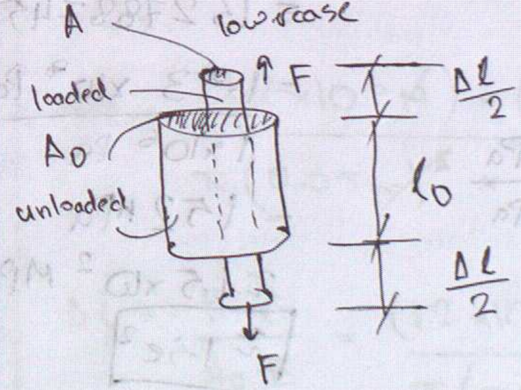
seems like diff k's and diff properties

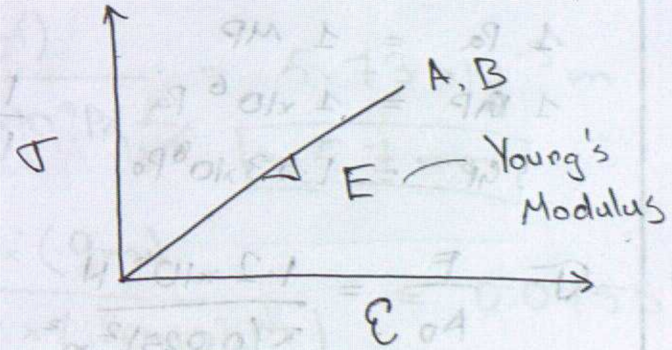
- Force and displacement not good way to characterize material properties

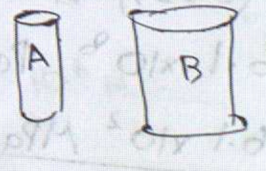
Engineering Stress and Stain

Stress : $\boxed{\sigma = \frac{F}{A_0}}$ "Sigma" lowercase

Strain: $\boxed{\varepsilon = \frac{\Delta l}{l_0}}$ "Epsilon"







$$\boxed{\sigma = E \varepsilon}$$

Hooke's Law (in tems of stess and strain)

Q.2.2.1 $E = 69\text{ GPa}$, $\sigma = \overset{60}{\wedge}\text{kPa}$, $\varepsilon = ?$

$\sigma = E\varepsilon \Rightarrow \varepsilon = \dfrac{\sigma}{E} = \dfrac{69\text{ GPa}}{60\text{ kPa}} = 1.15 \approx 1.2$

$\varepsilon = \dfrac{60\times10^3\text{ Pa}}{69\times10^9\text{ Pa}}$

$= \dfrac{69\times10^9\text{ Pa}}{60\times10^3\text{ Pa}} = 1150000$

$\approx 1.2\times10^6$

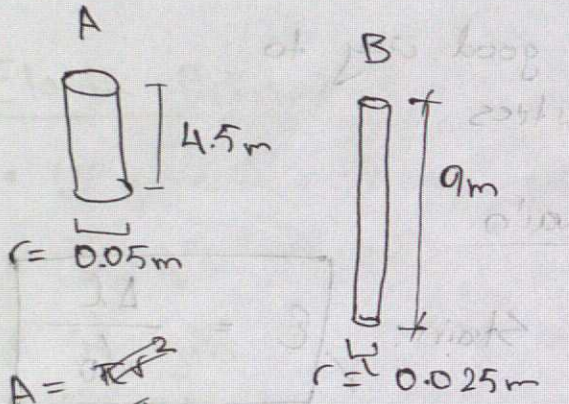
$\approx 1.2e^6$

$= 0.00000087$

$\approx 8.7\times10^{-7} = \boxed{8.7e^{-7}}$

Q.2.3.1

a)



$A = \cancel{\pi r^2}$
$= \cancel{\pi d}$
πr^2

$F = 1.2\text{ MN} = 1.2\times10^6\text{ N}$

$E = 120\times10^9\text{ Pa}$

$\boxed{\sigma = \dfrac{F}{A_0}} = \dfrac{1.2\times10^6\text{ N}}{\pi(0.05)^2\text{ m}^2}$

$= \cancel{1.53}$ N/m²

$= 152788745\text{ Pa}$

$= \dfrac{1.53\times10^8\text{ Pa}}{1\times10^6\text{ Pa}}$

$= 152\text{ MPa}$

$\approx 1.5\times10^2\text{ MPa}$

$\boxed{\approx 1.5e^2}$

$1\text{ Pa} = 1\dfrac{\text{N}}{\text{m}^2}$

$1\text{ Pa} = 1\text{ MP}$

$1\text{ MP} = 1\times10^6\text{ Pa}$

$?\text{ GP} = 1.53\times10^8\text{ Po}$

$\dfrac{1\times10^8\text{ Pa}}{1\times10^6\text{ Pa}}$

b) $\sigma = \dfrac{F}{A_0} = \dfrac{1.2\times10^6\text{ N}}{\pi(0.025)^2\text{ m}^2}$

$= 6.1\times10^8\text{ Pa}$

$= 6.1\times10^2\text{ MPa}$

$\boxed{= 6.1e^2\text{ MPa}}$

Q.2.3.1

c) $\varepsilon = \dfrac{\Delta l}{l_0}$, Δl in mm of bar A

stress $\sigma_A = 1.5\times10^2\text{ MPa}$
$= 1.5\times10^8\text{ Pa}$

$\sigma = E\varepsilon$

$\varepsilon = \dfrac{\sigma}{E} = \dfrac{\Delta l}{l_0} \Rightarrow \Delta l = \dfrac{\sigma}{E}\times l_0$

$\Delta l = \dfrac{1.5\times10^8\ \cancel{\text{N}}}{1.2\times10^6\ \cancel{\text{N}}\cdot\text{m}^{2}}\times4.5\cancel{\text{m}} = \dfrac{1.5\times10^8\text{ Pa}}{1.2\times10^6\text{ N}}\times4.5\text{m}$

~~$= \dfrac{562.5}{1\text{m}} = 0.0018\text{m} = \boxed{1.8\text{ mm}}$~~

~~$= \dfrac{1.5\times10^8\text{ Pa}\times4.5\text{m}}{69\times10^9\text{ Pa}} =$~~

$\dfrac{\frac{\text{N}}{\text{m}^2}}{\text{N}} = \dfrac{\text{N}}{\text{m}^2}\div\text{N}$

$= \dfrac{\cancel{\text{N}}}{\text{m}^2}\times\dfrac{1}{\cancel{\text{N}}}$

$= \dfrac{\cancel{\text{m}}}{\cancel{\text{m}^2}}$

$\dfrac{1}{\text{m}}$

c) $\sigma = \dfrac{F}{A_0}$ $\varepsilon = \dfrac{\Delta l}{l_0}$, $\sigma = E\varepsilon \rightarrow \varepsilon = \dfrac{\sigma}{E}$

$\dfrac{\Delta l}{l_0} = \dfrac{\sigma}{E}$ $\Delta l = \dfrac{\sigma\times l_0}{E} = \dfrac{F\ l_0}{A_0\ E}$

$\Delta l = \dfrac{(1.2\times10^6\ \cancel{\text{N}})\times(4.5\cancel{\text{m}})}{\pi(0.05\cancel{\text{m}})^{\cancel{2}}\times120\times10^9\text{ Pa}\frac{\cancel{\text{N}}}{\cancel{\text{m}^2}}} = 5.73\times10^{-3}\text{ m}$

$\boxed{= 5.7\text{ mm}}$

d) $\Delta l = \dfrac{F\cdot l_0}{A_0\cdot E} = \dfrac{(1.2\times10^6\ \cancel{\text{N}})\times(9\text{m})}{\pi(0.025\cancel{\text{m}})^{\cancel{2}}\times(120\times10^9\ \frac{\cancel{\text{N}}}{\cancel{\text{m}^2}})} = 0.0458\text{m}$

$= 45.8\text{ mm}$

$\boxed{\approx 46\text{ mm}}$

e) $r_A = 0.05$, $l_{0A} = 4.5\text{m}$, $F_A = 1.2\times10^6\text{ N}$

$E = 120\times10^9\text{ N/m}^2$

$\sigma_A = \dfrac{F_A}{A_{0A}} = \sigma_B = \dfrac{F_B}{A_{0B}} \Rightarrow \dfrac{F_A}{A_{0A}} = \dfrac{F_B}{A_{0B}} \Rightarrow \dfrac{F_A\times A_{0B}}{A_{0A}} = F_B$

$F_B = \dfrac{(1.2\times10^6\text{ N})\times(\pi(0.025\cancel{\text{m}})^2)}{(\pi(0.05\cancel{\text{m}})^2)} = 300000\text{ N}$

$= 300\text{ kN} = 3\times10^3\text{ kN}$

$\boxed{3e^3}$

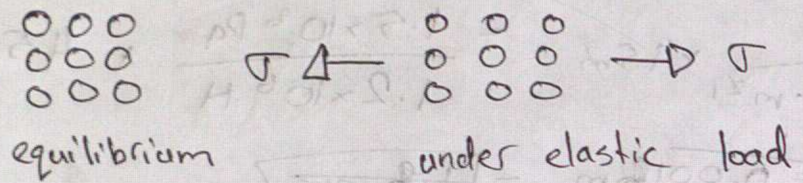
Elastic Behaviour

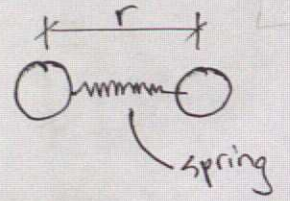
June 6,23

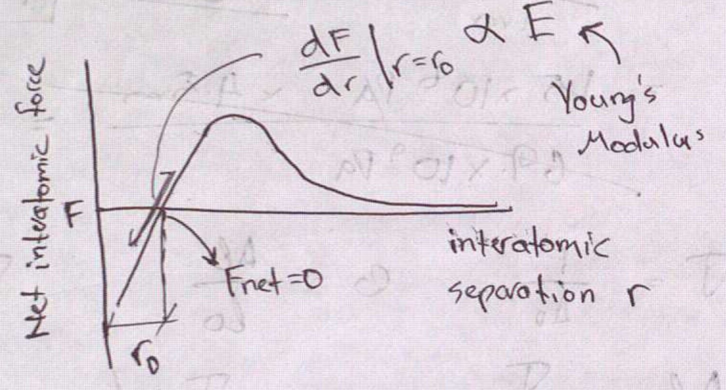
Defining Elastic Deformation

1) During elastic deformation, atoms return to their original position upon unloading

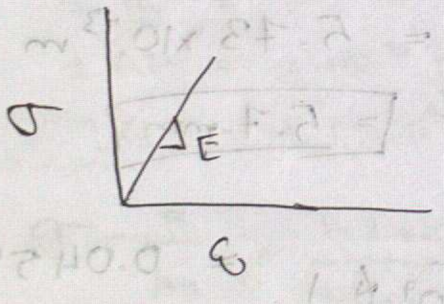
Bonding for Solids







Stucture Independence of Young's Modulus



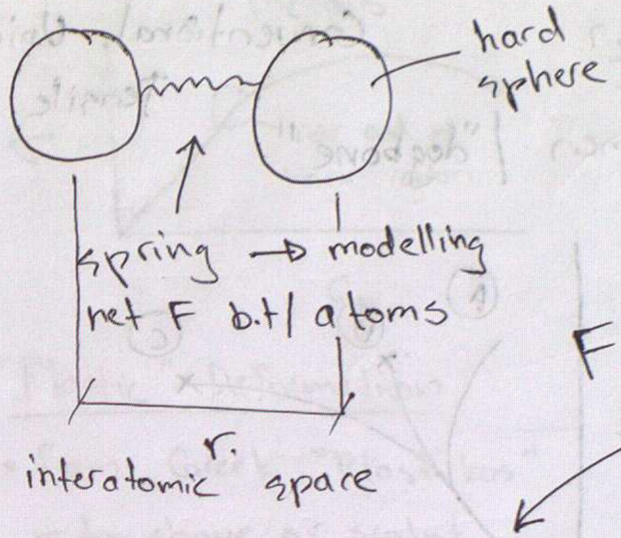
what is elastic ?

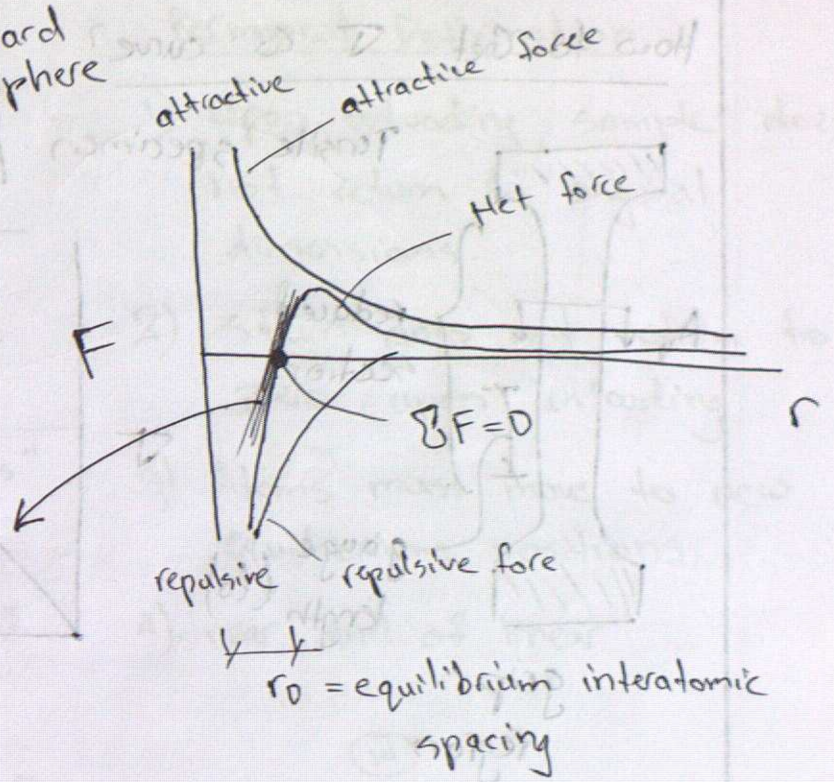
1) sample returns to original geometry upon unloading
2) strain is recoverable

→ 3) Atoms also return to origial posit. upon unloading

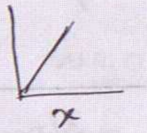
Elastic Behaviour

June 6,23





slope = $\frac{dF}{dr}$ =



Young's Modulus

$$\boxed{E \propto \frac{dF}{dr}\Big|_{r=r_0}}$$

important caz tells us E depends only on type of atoms

→ Young's Modulus is <u>sturcture independent</u>

Eg

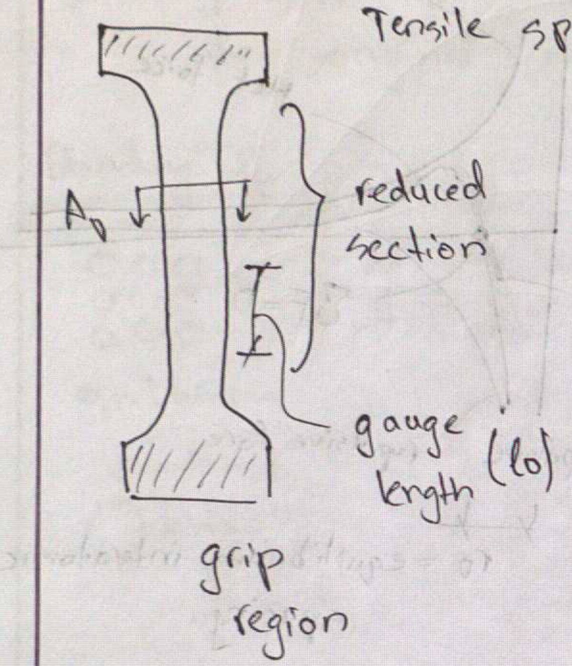
- Small changes to composition (concentration) do not change Young's Modulus, nor does strengthening

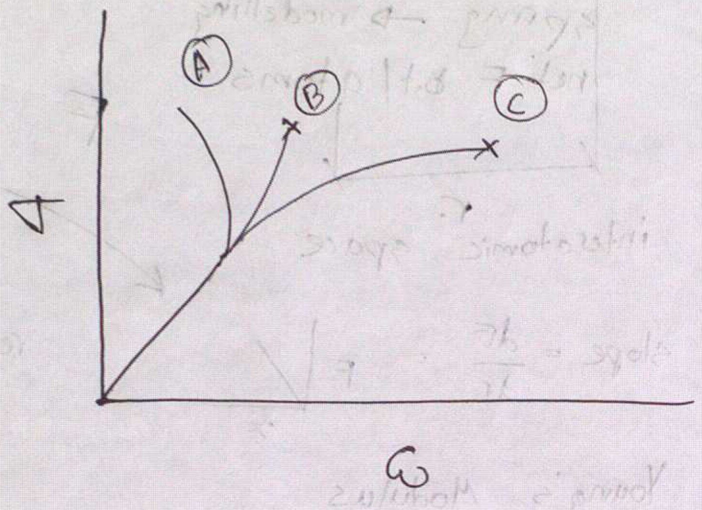
Elastic Behaviour June 6, 23

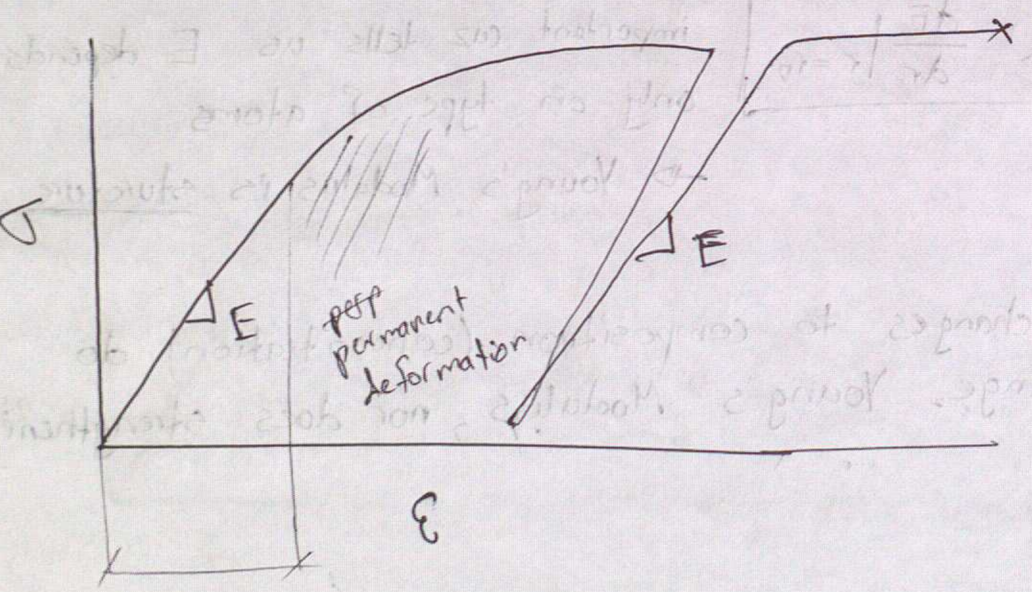
How to Get σ - ε curve?

Conventional Uniaxial Tensile Test

Tensile specimen / "dogbone"





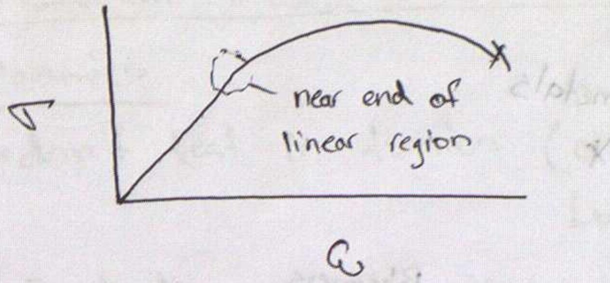


Summary

- Elastic deformation involves atoms moving slightly away from each other
- Young's Modulus describes elastic behaviour

Behaviour That's Not Elastic June 7, 23

Metals



"Plastic" Deformation

- from Greek "Plastikos"
  - to shape or sculpt
- same as plastic surgery
- permanent deformation

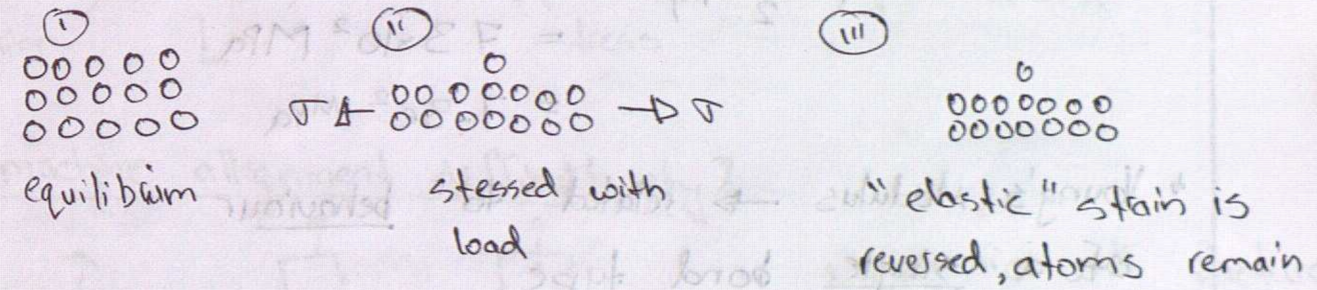
Permanent Deformation

1) Upon unloading, sample does not return to original dimensions.

2) Strain does not return to zero upon unloading

3) Atoms must move to new equilibrium positions

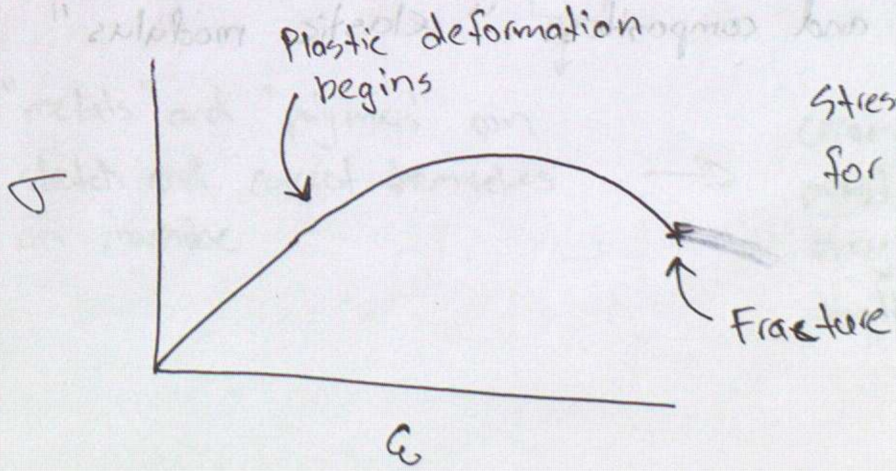
A) near end of linear



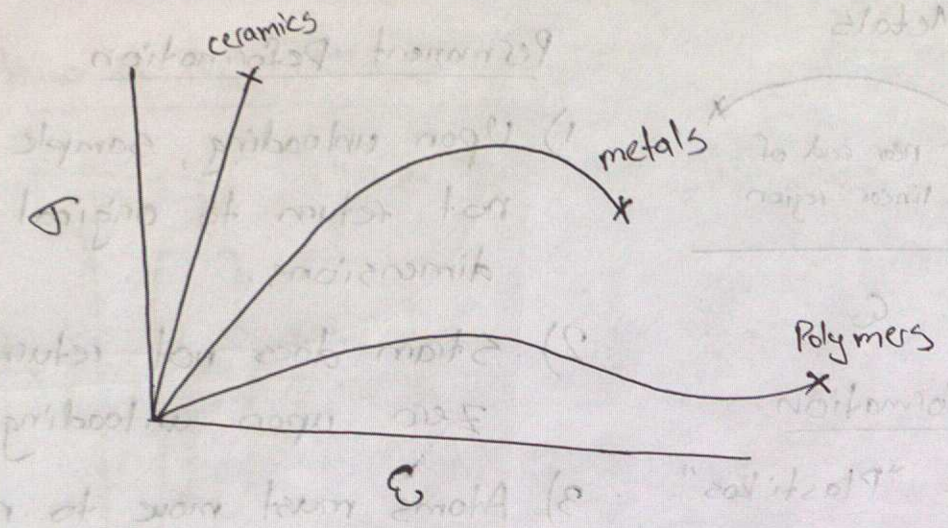
3.1.1 $\varepsilon = 0.001$, $\sigma = ?$ in MPa!

$$\sigma = E\varepsilon$$

$$= (200 \times 10^9) \times 0.001 = 2.0 \times 10^8 \text{ Pa} = \boxed{2.0 \times 10^2 \text{ MPa} \approx 2e^2}$$



Stress-Strain Curve for metal



Q.3.3.1 $F = 83 \times 10^3\ N$, $d = 12\ mm = 0.012 m$, $\sigma = ?$

$$\sigma = \frac{F}{A_0} = \frac{83 \times 10^3\ N}{\pi\left(\frac{0.012}{2} m\right)^2} = 7.3 \times 10^8\ Pa$$

$$= 7.3 \times 10^2\ MPa$$

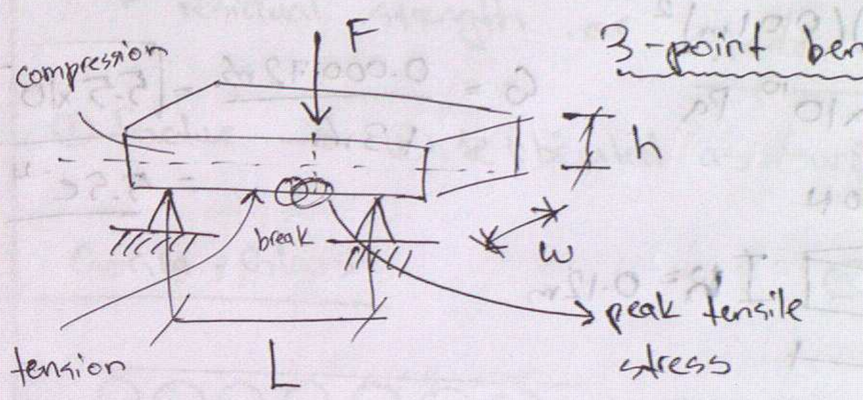
$$= 7.3e^2\ MPa$$

- Young's Modulus → related to <u>behaviour</u> of a <u>single</u> bond type
- Elastic response of polymers depends on many primary and secondary bonds
- For polymers and composites: "elastic modulus"

Mechanical Behaviour of Other Materials

Ceramics

- don't test in tension (crumbles in grip, difficult to machine)
  ↳ machine allignment difficult *
- Instead, we load with bending

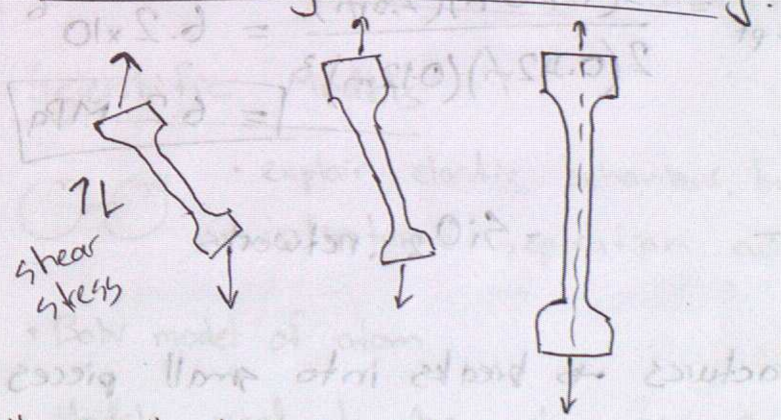


3-point bending

$$\boxed{\sigma_{3\text{-point}} = \frac{3FL}{2w \cdot h^2}}$$

peak stress

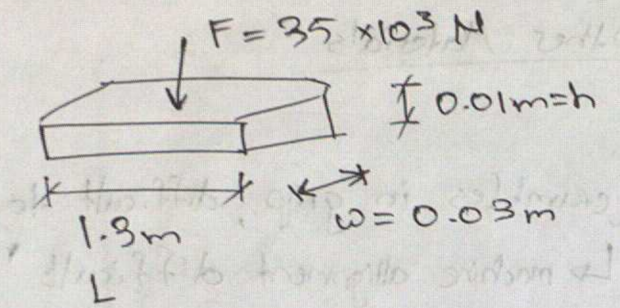
* machine allignment difficult why?



- ceramic will fracture at very low value of strain

"metals" and "polymers" can stetch and correct themselves on machine → ceramics can't undergo plastic deformation since they're brittle and will shatter.

3.3.2



$\Delta l = 0.72\,mm = 0.00072\,m$

$\varepsilon = \frac{\Delta l}{l_0}$ $\sigma = \frac{F}{A_0}$

$\sigma_{3\text{-}pt} = \frac{3FL}{2w \cdot h^2}$ $\sigma = E\varepsilon$

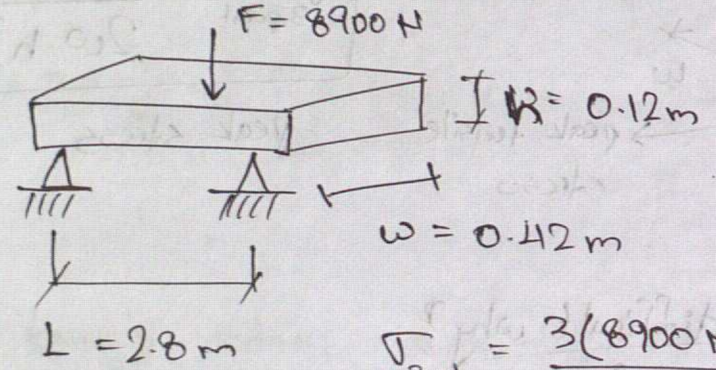
$$\sigma_{3\text{-}pt} = \frac{3(35 \times 10^3 N)(1.3\cancel{m})}{2(0.03\cancel{m})(0.01m)^2}$$

$$= 2.275 \times 10^{10}\ Pa$$

$$\varepsilon = \frac{0.00072\cancel{m}}{1.3\cancel{m}} = \boxed{5.5 \times 10^{-4}}$$

$$= \underline{5.5e^{-4}}$$

3.13.1



$$\sigma_{3\text{-}pt} = \frac{3(8900\,N)(2.8\cancel{m})}{2(0.42\cancel{m})(0.12m)^2} = 6.2 \times 10^6\ Pa$$

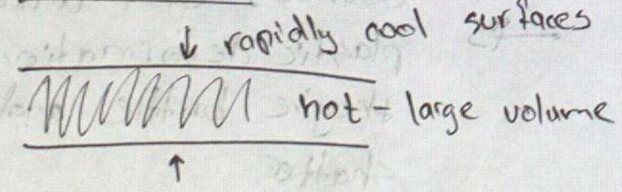
$$\boxed{= 6.2\ MPa}$$

Tempered Glass

- high strength
- "safe" when fractures → breaks into small pieces

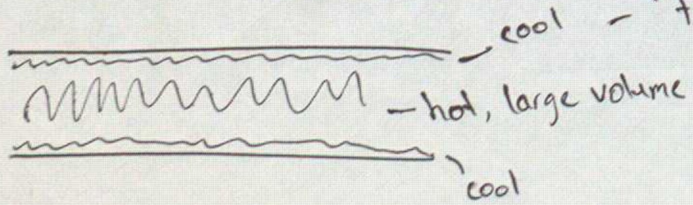
- SiO₂ networks

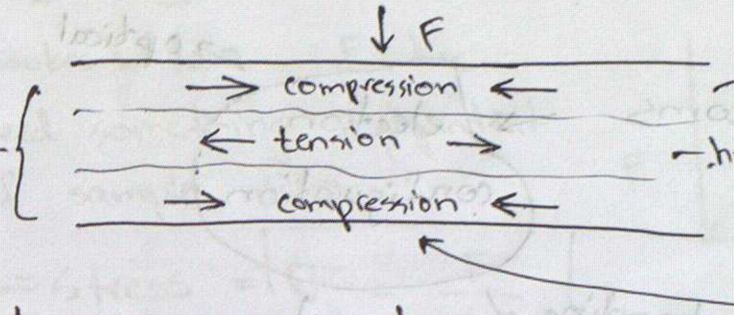
cross-section

① 

} also with chemical process
↳ Gorilla glass

"frozen-in" exess volume

② 

③ 

- cool - "frozen-in" excess volume

- hot, larger volume

* tempered glass's stength

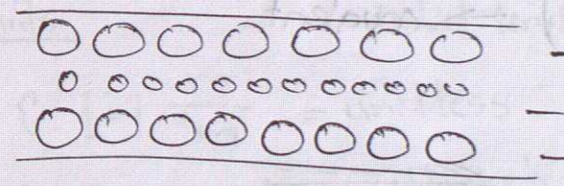
- lower glass side starts in compression to begin with

* ceramics good at compression

→ residual strength, or Stored Strain Energy

① fracture → ⑪ be liberated as surface energy
↓
⑪ small pieces

Gorilla - Glass



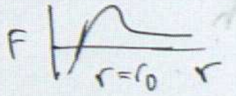
— exta space — increase volume — compresive

— tensile

— compresive

Scientific Models

- explain elastic behaviour, but not permanent deformation
- interatomic separation curve



- Bohr model of atom
- Models need to be only as good to explain the current matter
- Models with limitations → What's the Point?
  ↳ good at explaining certain things
- You don't need models if you already understand everything perfectly.

Intro & Hooke's Law – 01

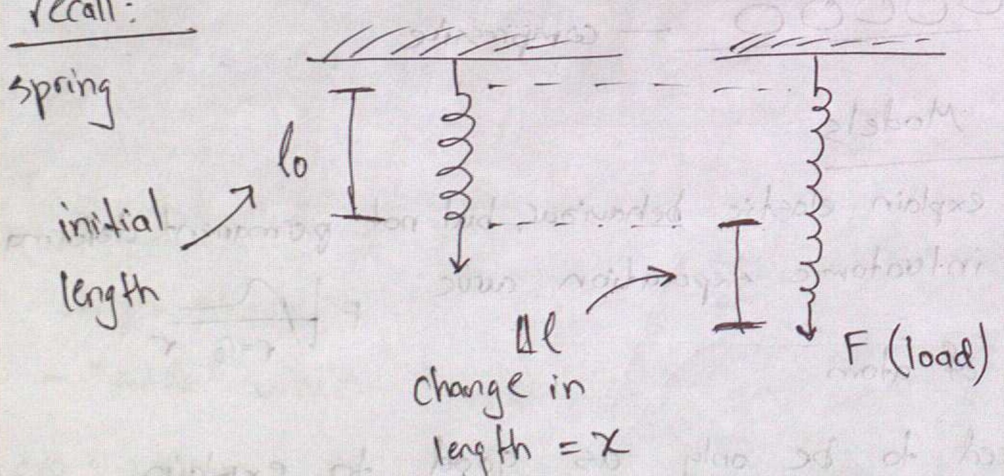
Mechanial Behaviour → atoms → electron configuration → optical

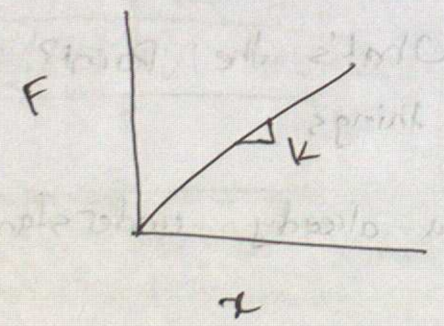
bonding ↙ electrical ↓

Classify All Material

- Metals (eg. Fe, Au, Al, Cu) → metallic bonding
  ↓ band theory of solids
- Ceramics (eg. Porcelain) → ionic
- Polymer (eg. PVC, "plastics") → covalent

recall:



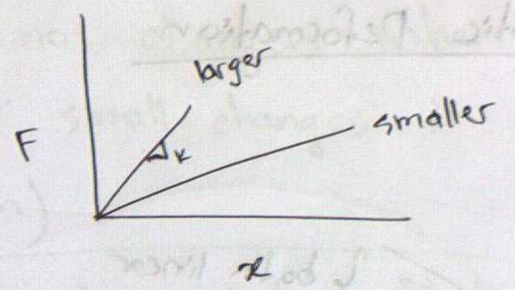


$\boxed{F = kx}$

force, elongation, spring constant

Engineering Stress and Strain – 02

- Hookes's law $F = kx$
- need something independent of sample size

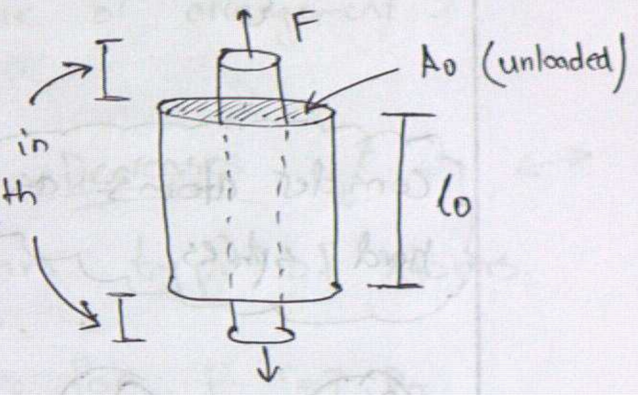


⇒ Stress = $\boxed{\sigma = \frac{F}{A_0}}$ ← initial cross-sectional area

"sigma"

units:

$\sigma\ [=]\ \frac{N}{m^2} = Pa$



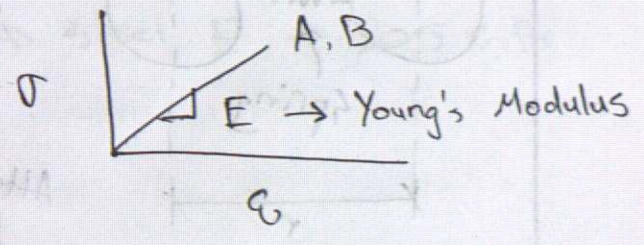
⇒ Strain = $\boxed{\varepsilon = \frac{\Delta l}{l_0}}$ ← change in length

↑ initial length

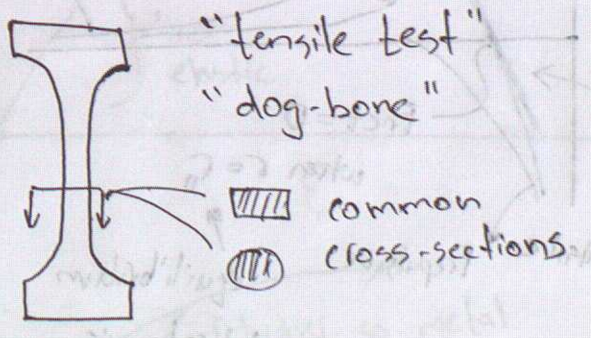
units

$\varepsilon\ [=]\ \frac{m}{m}$ = unitless

$\boxed{\sigma = E\varepsilon}$ Hooke's Law

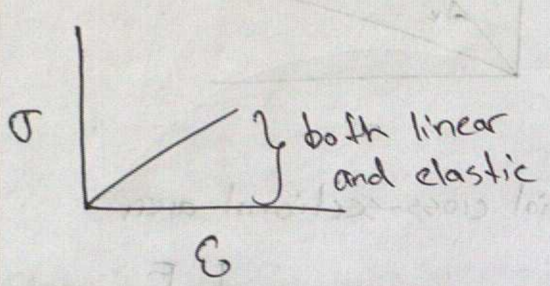


Uniaxial Tension



Engineering Stress and Strain - 02

Elastic Deformation

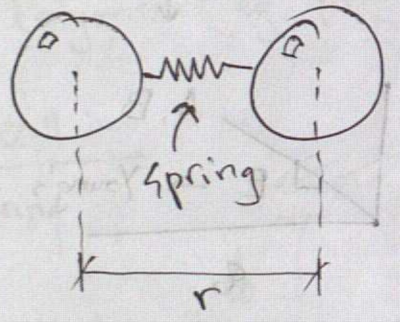


→ Strain is restored or recovered

→ Sample dimensions return to original upon unloading

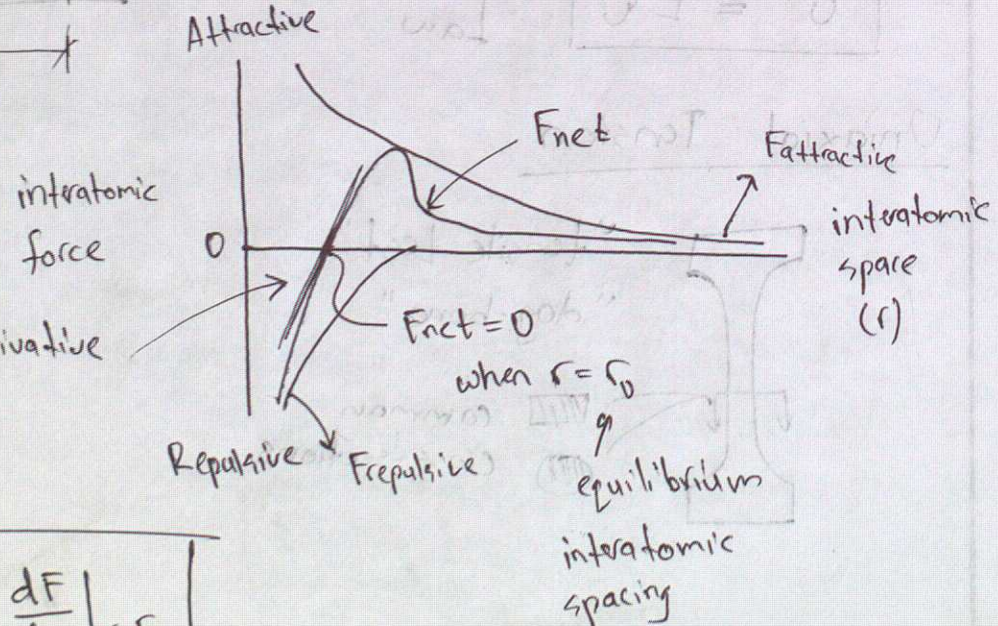
→ atoms return to original positions

Consider atoms as hard spheres



Mechanical model for interatomic models

"if you know everything, you don't even need models"



slope or 1st derivative

$$\frac{dF}{dr}$$

$$\boxed{E \propto \left.\frac{dF}{dr}\right|_{r=r_0}}$$

Young's Modulus

directly proportional to

equilibrium spacing

Atomic Definition, Tensile Testing - 03

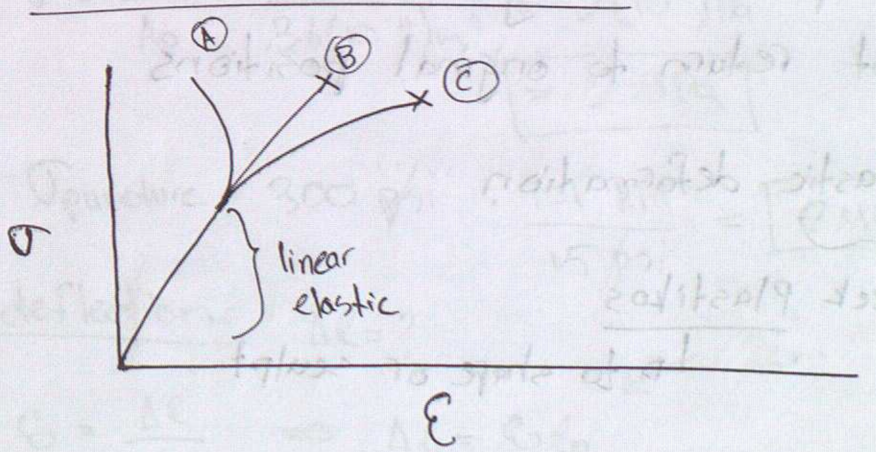
- Young's modulus does not changen when the strength changes or for small changes in composition (concentration)
- Young's Modulus is $\boxed{\text{structure - independent}}$ → microstructure or arrangement of atoms
- Heat metal → Young's Modulus <u>Decreases</u> ↕ ⇒ ↔
- Young's Modulus depends only on type of atoms.

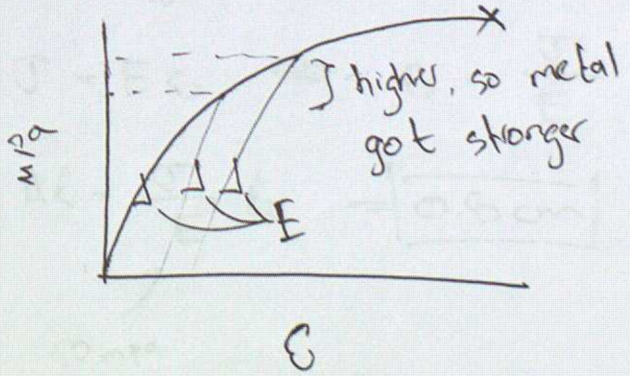
$$E.\ [=]\ \frac{Pa}{m/m} = Pa$$

units for E [=]. Pa

↳ steel E = 205 GPa

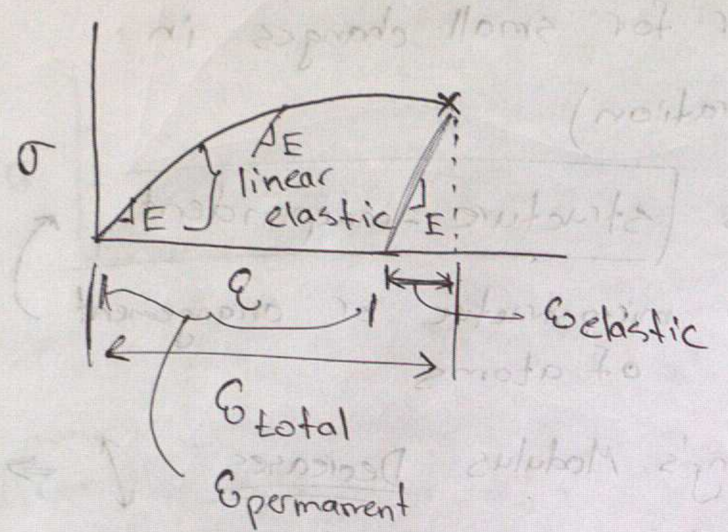
After Elastic Deformation





Pastic Deformation, Bed of Nails -04

Metals



How to define permanent deformation?

1) close to end of linear region
2) sample does not return to original dimensions upon unloading
3) atoms do not return to original positions

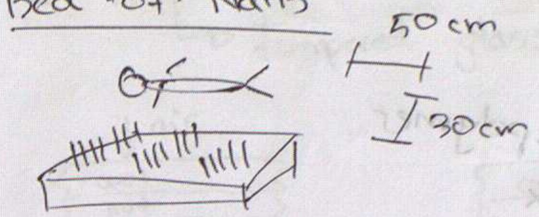
Permanent = Plastic deformation

$\underbrace{\text{Plastic}}$ Greek Plastikos

↳ to shape or sculpt

Plastic Deformation, Bed of Nails -04

Bed - of - Nails



• sharpness of nails

$D \approx 15\,\text{mm} = 1.5(10^{-3})$

(diameter)

$\sigma = \frac{F}{A_0}$

$F = 80\,\text{kg} \times 9.8 \frac{N}{kg}$

$= 800\,N$

$A = \frac{\pi D^2}{4} \cdot n_{nails} \approx \frac{3}{4}\, 2.25\,(10^{-3})^2 = \frac{6}{4} 10^{-6}$

$= \frac{6}{10} 10^{-6} \cdot n_{nails}$

$= \frac{6}{4}\, 240(10^{-6})$

$= 3.6(10^{-4})\,m^2$

$n_{nails} = \frac{\text{width}}{\left(\frac{\text{lin}}{\text{nail}}\right)} \frac{30\,\text{cm}}{\frac{2.54\,\text{cm}}{\text{in}}} = 12$ nails

length = 20 nails

n.nails = (20 x 12) = 240

$\sigma = \frac{F}{A_0} = \frac{800\,N}{3.6(10^{-4})\,m^2} = 2(10^6)\,Pa$ $\boxed{= 2\,MPa}$

$\sigma_{puncture} = 300\,\text{psi} \cdot \frac{101\,kPa}{15\,\text{psi}} = \boxed{2\,MPa}$

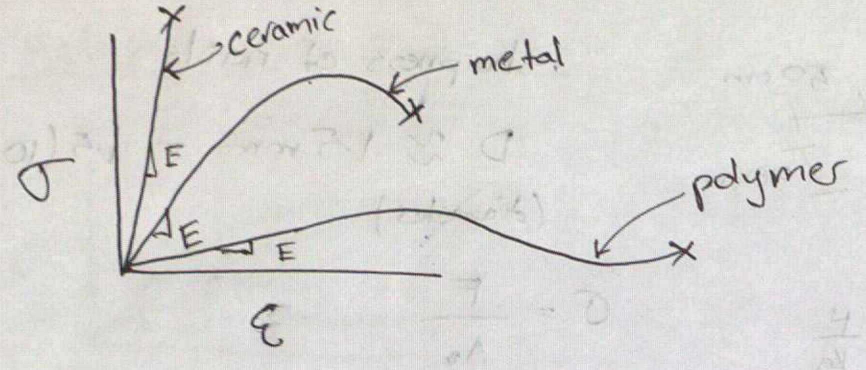
deflection $\Delta l = ?$ ↙ 2cm

$\varepsilon = \frac{\Delta l}{l_0} \Rightarrow \Delta l = \varepsilon l_0$

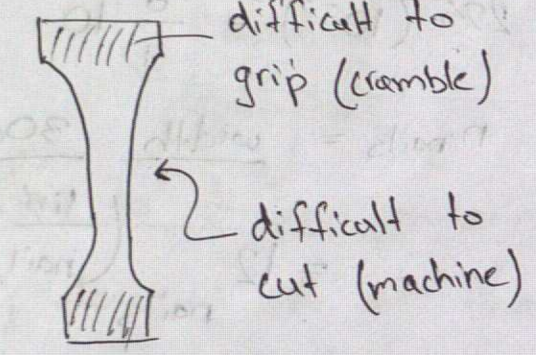
$\sigma = E\varepsilon \Rightarrow \varepsilon = \frac{\sigma}{E}$

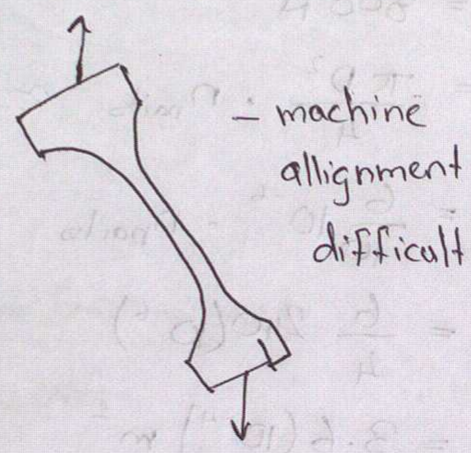
$\Delta l = \frac{\sigma}{\underset{\nearrow\,50\,mpa}{E}} l_0 = \boxed{0.8\,cm}$

3-Point Bend Testing, Modulus Vs. Density -05



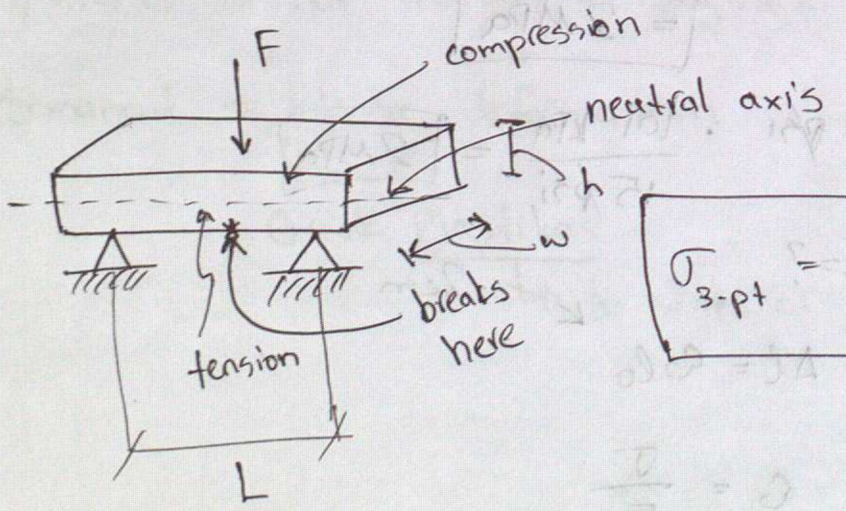
How to test Ceramics





Bend Test

3-point bend test

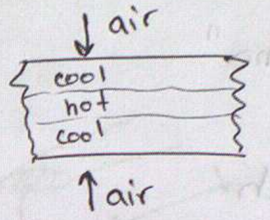


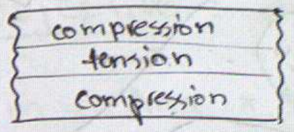
$$\boxed{\sigma_{3\text{-pt}} = \frac{3FL}{2wh^2}}$$

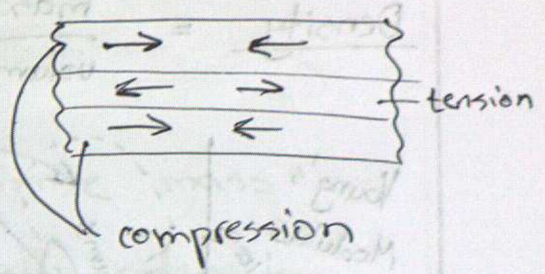
3-Pt bend Test. Modulus vs. Density -05

eg: Glass shelf

↳ tempered glass







Glass Standing

$m = 80$ kg

$L = ?$

$h = 4.5$ mm

$w = 15$ ~~mm~~ cm

$$\sigma = \frac{3FL}{2wh^2}$$

$$L = \frac{2\sigma wh^2}{3F}$$

$w = 15\text{ cm} = 15(10^{-2})\text{m}$

$h = 4.5\text{mm} = 4.5(10^{-3})\text{m}$

$F \approx 800\text{N}$

$\sigma_{fracture} = 120(10^6)\text{Pa}$

$$L = \frac{2(120(10^6))(15(10^{-2}))(4.5\times10^{-3})^2}{3(800)} = 0.30\text{m} = \boxed{30\text{ cm}}$$

2) $h = 2\text{mm} = 2\times10^{-3}\text{m}$

$\boxed{\text{Gorilla Glass}}$

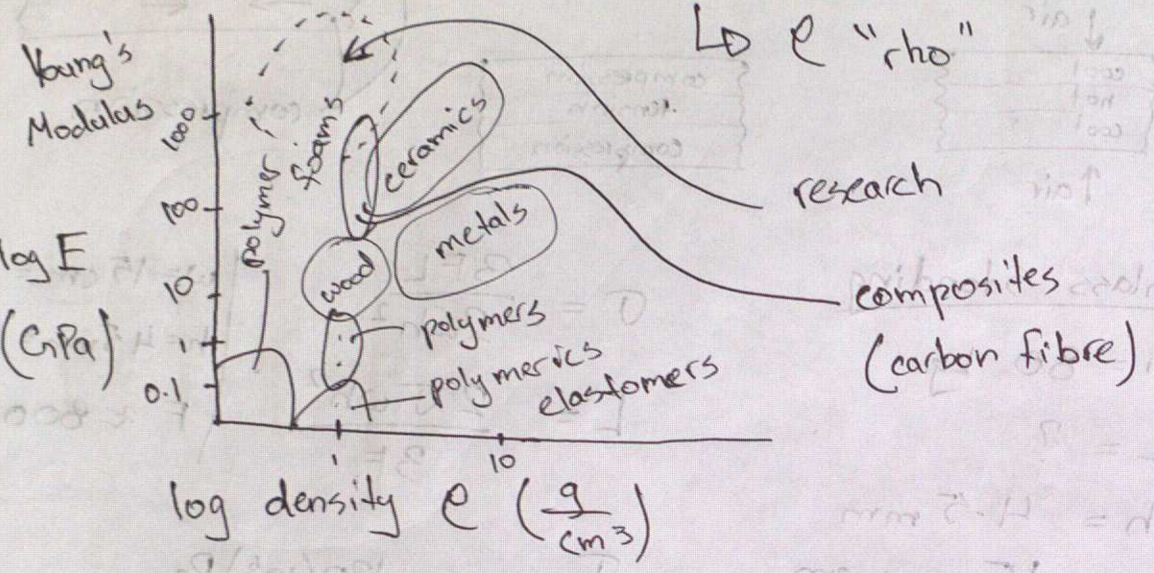
$\sigma_{fracture} = 300(10^6)\text{Pa}$

$$L = \frac{2(300\times10^6)(15\times10^{-2})(2\times10^{-3})^2}{3(800)} = 0.15\text{m} = \boxed{15\text{ cm}}$$

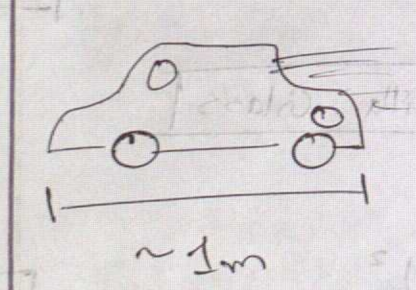
Density - 05

Density $= \frac{\text{mass}}{\text{volume}} \; [=] \; \frac{g}{cm^3}$ or $\frac{kg}{m3}$

↳ ρ "rho"



* E_{metals} → 100s of GPa



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4 - Structure - Property Relationship

Helicopter Rotor

* rotor is loaded in bending

objective : minimize mass

m = Area × length × density

$$\boxed{m = A \cdot L \cdot P}$$

↳ density ρ "rho"

Constraint: maximum deflection

$$\boxed{\delta = \frac{FL^3}{CEA^2}}$$

deflection

Young's Modulus

Area

* isolate for area

$$A = \sqrt{\frac{FL^3}{CE\delta}}$$

} put into origial objectiv

$$m = ALP$$

$$= \left(\frac{FL^3}{CE\delta}\right)^{1/2} \cdot L \cdot \rho$$

material properties

* minimize $\frac{\rho}{E^{1/2}}$

OR

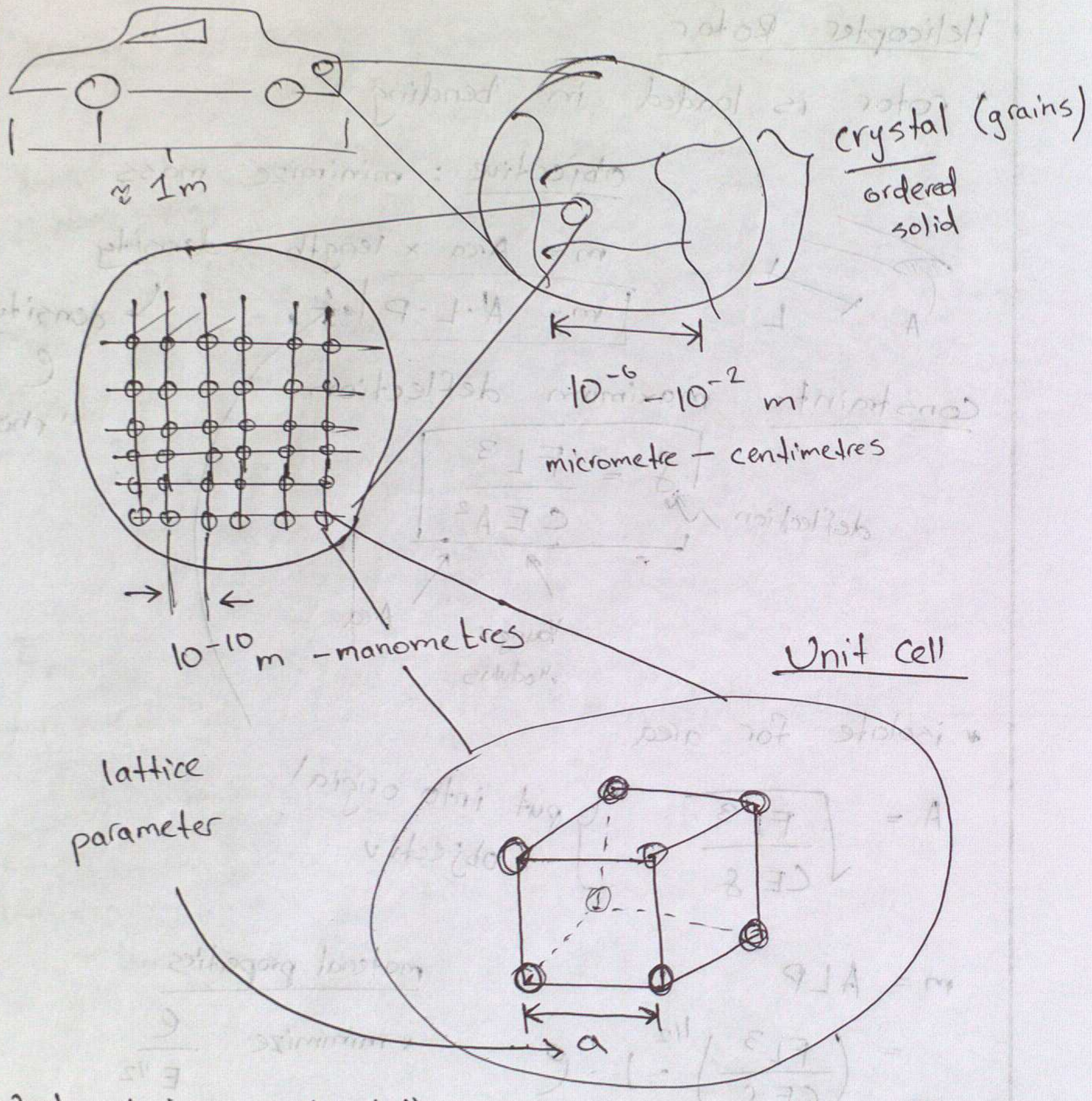
* maximize $\frac{E^{1/2}}{\rho}$ } material performance index (MPI)

– $MPI = \frac{E^{1/2}}{\rho}$

$$\log MPI = \frac{1}{2}\log E - \log \rho$$

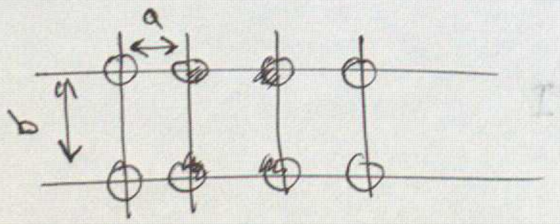
$$\log E = 2\log \rho + 2\log MPI$$

Face-Centered Cubic -06



- Unit cell is smallest "convenient building" block" that describes structure → polycrystaline

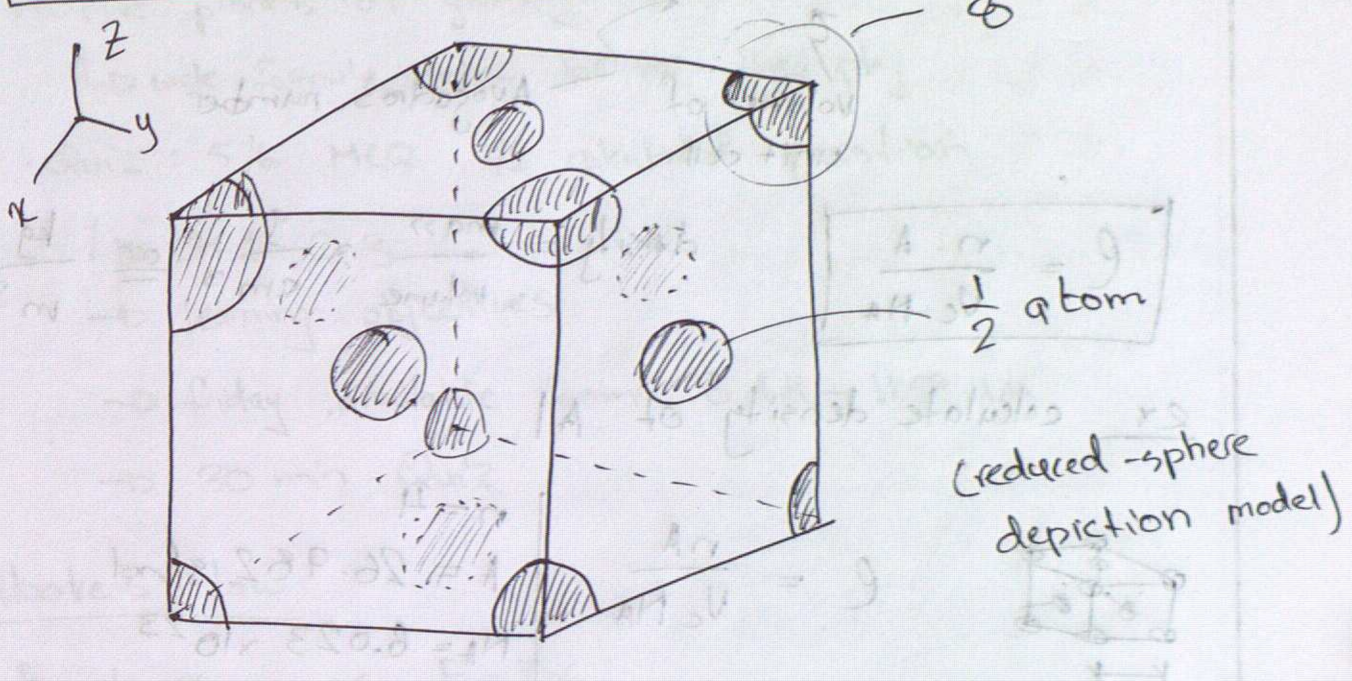
Eg unit cell in 2D: students in class



Face-centered Cubic -06

- An important crystal structure (ex: Al) many metals

Face-centered Cubic (FCC)



- Number of atoms in FCC unit cell ↳ 4 atoms

$$\frac{1}{8} \times 8 = 1$$

$$\frac{1}{2} \times 6 = 3$$

$$\boxed{n_{FCC} = 4}$$

Density - 06

density = $\frac{\text{mass}}{\text{volume}}$

molar mass

$$\text{"rho"} \rightsquigarrow \rho = \frac{n \cdot A}{V_c N_A} \;[=]\; \frac{\cancel{\#} \cdot g/\cancel{mol}}{m^3 \cdot \cancel{N_A}/\cancel{mol}} = \frac{g}{m^3}$$

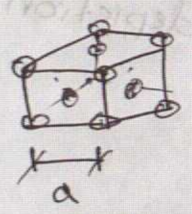
volume of unit cell

Avogadro's number

$$\boxed{\rho = \frac{n \cdot A}{V_c \cdot N_A}}$$

density = $\frac{\text{mass}}{\text{volume}} = \frac{g}{cm^3}$ or $\frac{kg}{m^3}$

<u>ex</u> calculate density of Al



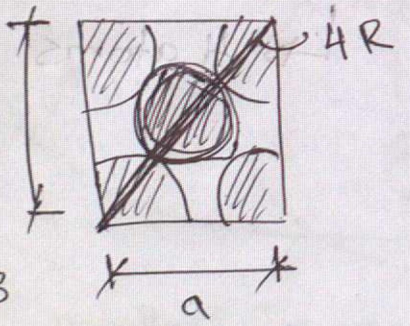
$$\rho = \frac{nA}{V_c N_A}$$

$n = 4$
$A = 26.982$ g/mol
$N_A = 6.023 \times 10^{23}$
$R = 143 \times 10^{-12}$ m

$V_c = a^3$

$\downarrow$

$V_c = (2\sqrt{2}R)^3$



$a^2 + a^2 = (4R)^2$

$2a^2 = 16R^2$

$a = 2\sqrt{2}R$

$$\rho = \frac{nA}{(2\sqrt{2}R)^3 N_a} \;[=]\; \frac{\cancel{\#} \cdot g/\cancel{mol}}{m^3 \cdot \cancel{\#}/\cancel{mol}} = \frac{g}{m^3}$$

$$= \frac{4(26.982)}{(2\sqrt{2}(143 \times 10^{-12}))^3 (6.023 \times 10^{23})}$$

$$= 2.7 \times 10^6 \; g/m^3 \cdot \left(\frac{1m}{100cm}\right)^3 = \boxed{2.7 \; g/cm^3}$$

Tutorial #1

Wed, Jul 12, 23

About Her

- Diana : d.rakotonirina@mail.utoronto.ca
- Take care of units
- Write process of getting answers
  - ↳ write formula, solve for var, the plug
- Quiz : 5/6 MCQ. 1/2 calculated question
  - ↳ Ch. 1, 2, 3
  - → learning objectives
  - → friday, available from 8 AM – 11:59 AM
  - → 30 min Quiz

Hooke's Law

$F \propto x$ or $F = kx$

- Fapp is proportional to the distance stretched

Tension

- Force applied when material stretched
- Tensile strength (how good material performs [doesnt fracture] under tension) metals, polymers

Tutorial #1

Tensile strength: Young's Modulus

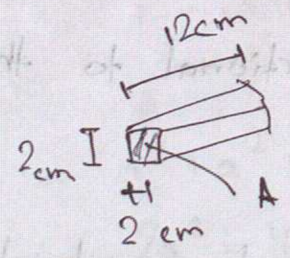
- Slope of stress-strain curve
- $E = \frac{\sigma}{\varepsilon}$
  - → σ is ~~strain~~ stress (Pa)
  - → ε is strain (unilless)
  - → E (Pa)
- E gives force required to induce certain deformation
- lower E = more elastic

Hooke's Law v.s. E

- k depends on geomefy
- E is geomefy-independent

Stress

F, force   A, area



- $\sigma = \frac{F}{A} = \frac{N}{m^2} = Pa$

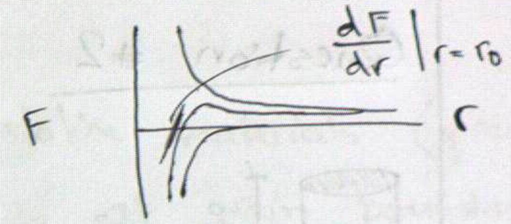
Strain

$$\varepsilon = \frac{\Delta l}{l_0} = \frac{l_{final} - l_{initial}}{l_{initial}} \quad [=] \quad \frac{m}{m} = \text{unilless}$$

$$\frac{0.006m}{3m} = 0.002 \text{ or } 0.2\%$$

Tut #1

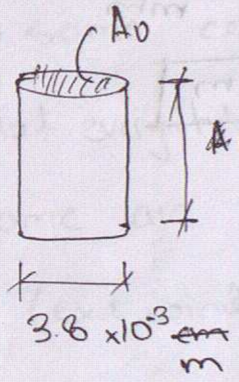
Atomic level



- E_p in atom bonds
- r = elongation
- at some point r_0, $F_{attrac.} = F_{repuls}$, so $\Sigma F = 0$

$$\boxed{\frac{dF}{dr} \propto E} \qquad \frac{dF}{dr}\Big|_{r=r_0} \propto E$$

Question #1



$E = 107 \times 10^9$ Pa

$F = 2000$ N

$\Delta l = 0.42 \times 10^{-3}$ m

$l_{max} = l_0 + \Delta l$

$\sigma = E \varepsilon$

$\frac{F}{A_0} = E \cdot \frac{\Delta l}{l_0}$

$F l_0 = E \Delta l A_0$

$l_0 = \frac{E \Delta l A_0}{F}$

$A_0 = \pi r^2$

$= \pi \left(\frac{3.8 \times 10^{-3}}{2}\right)^2$

$$l_0 = \frac{(107 \times 10^9 Pa)(0.42 \times 10^{-3} m)\left(\pi\left(\frac{3.8 \times 10^{-3} m}{2}\right)^2\right)}{2000N}$$

$= 0.255$ m

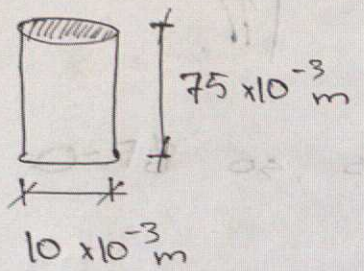
$\boxed{= 25.5 \text{ cm}}$

$l_{max} = 0.255 m + 0.42 \times 10^{-3} m$

$= 0.255 m$

Tutorial #1

Question #2



$F = 20{,}000 N$

$E = 200 \times 10^9 Pa$

$\Delta l = ? m$

$\sigma = E \varepsilon$

$\sigma = \frac{F}{A_0}$

$\varepsilon = \frac{\Delta l}{l_0}$

$$\frac{F}{A_0} = \frac{E \Delta l}{l_0} \Rightarrow \Delta l = \frac{F l_0}{A_0 E}$$

$$\Delta l = \frac{(20.000 N)(75 \times 10^{-3} m)}{\left(\pi \left(\frac{10 \times 10^{-3}}{2}\right)^2\right)(200 \times 10^9 Pa)} = 9.55 \times 10^{-5} m$$

$$= 9.55 \times 10^{-2} mm$$

$$\boxed{= 0.096 mm}$$

Structure - Property Relation - 04

Ordered Solids

- crystals that make up poly crystaline materials (grains)
- polished hand rail → eaten away at grain boundaries
- long range order (cubic symmetry, can extend for beyond)
- short range order (knowledge of only nearest neighbor atoms)

12 - FCC

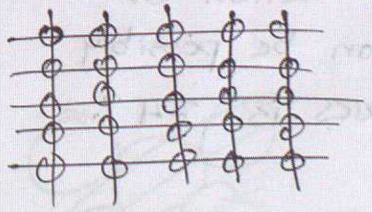
- most metals crystaline
- some ceramics (ex: Al_2O_3 - saphire) sapphire

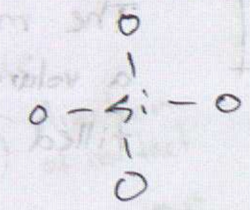
Not everything is crystaline!

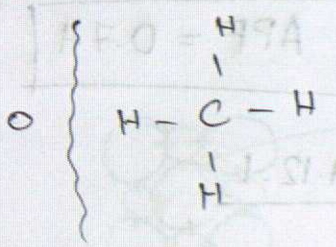
some are amorphous (not organized)

- (ex: window glass)

Long range order	VS.	short range order
well beyond nearest atoms		1st or 2nd nearest neighbor

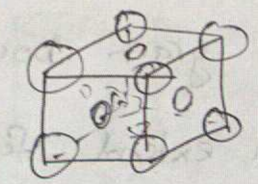






Density - TopHat

Q.4.10.1



$R = 184\ pm = 184 \times 10^{-12}\ m$

$A = 26.982\ g/mol$

$\rho = ?$

$\rho = \frac{nA}{V_C N_A}$

$\cancel{A_0 =}$

$\cancel{\rho = \frac{nA}{A_D N_A}}$

$V_C = (2\sqrt{2}R)^3$

$$\rho = \frac{nA}{(2\sqrt{2}R)^3 N_A} = \frac{4 \times 26.982\ g/mol}{(2\sqrt{2}(184\times10^{-12} m))^3 (6.023\times10^{23})} [=] \frac{g}{m^3}$$

$$= 1271255 \frac{g}{m^3} \times \left(\frac{1m}{100cm}\right)^3 = 1.27 \frac{g}{cm^3}$$

Atomic Packing Factor (for FCC)

$$APF = \frac{Volume_{sphere}}{Volume_{unit\ cell}} = \frac{n \cdot \frac{4}{3}\pi R^3}{a^3} = \frac{4 \frac{4}{3}\pi R^3}{a^3}$$

$$\text{Since } a^3 = (2\sqrt{2}R)^3 \Rightarrow APF = \frac{4\frac{4}{3}\pi R^3}{(2\sqrt{2}R)^3} = 0.74$$

$\boxed{\therefore APF = 0.74}$

The maximum fraction of a volume that can be possibly filled with spheres is 74%.

Q.4.12.1

$\frac{74}{100} = \frac{144.3 L}{195 L}$ $\approx$ 144 L of foam spheres

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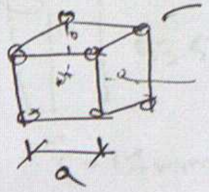
Rock Salt ceramic crystal - lec 07



$\frac{1}{8} \cdot 8 = 1$
$\frac{1}{2} \cdot 6 = 3$ } $n_{FCC} = 4$

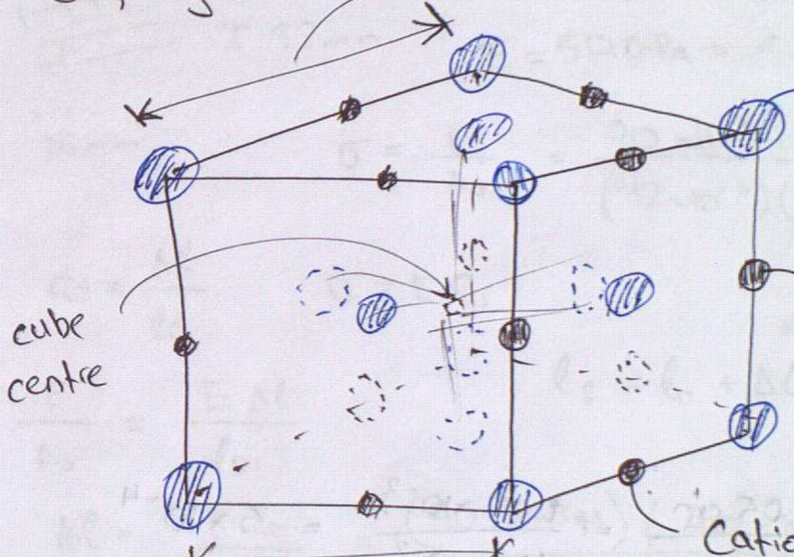
FCC - Face-centric cubic (many metals)

* Ceramic Structure

Rock Salt (NaCl)

FeO, MgO

$a = 2R_c + 2R_A$



Anions in "FCC-type positions"

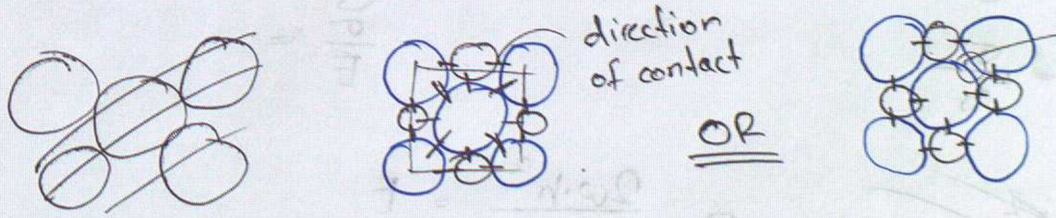
$\frac{1}{4}$ of atom × 12 edges
= 3 + ① cube centre
= 4

Cations in "edge-centered" positions

NaCl
1:1

Na Cl
4 : 4 } because anion in FCC

Front Face



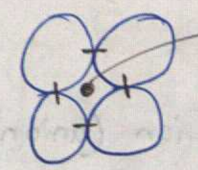
number of nearest neighbor atoms touching = $\boxed{\text{coordination number}}$ C.N.

$CN_{NaCl} = 6$

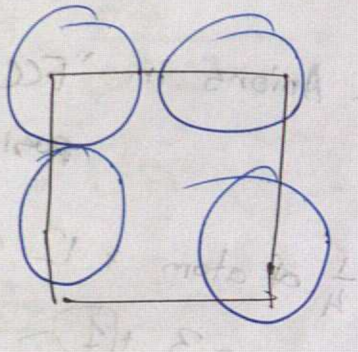
cations in rock salt ∴ occupy <u>octahedral interstital sites</u>

Rock Salt - Lec 06

This does NOT occur



Size of Octahedral site



Quiz #1

$\varepsilon = \frac{\Delta l}{l_0} = \frac{0.05\,cm}{100\,cm} = \frac{0.05 \times 10^{-2}\,m}{100 \times 10^{-2}\,m} = 5 \times 10^{-4}$

$\sigma = E\varepsilon$

~~$E = \frac{\sigma}{\varepsilon}$~~

$E = \frac{\sigma}{\varepsilon}$

a) ~~90000 Pa = 9~~

$\sigma = E\varepsilon$

$\frac{\sigma}{\varepsilon} = E$

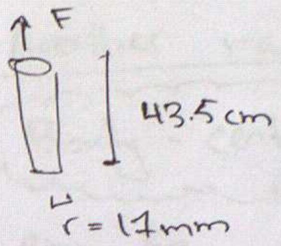
$\frac{\sigma}{E} =$

3. ~~$\square \frac{3\omega \cdot h^2}{3 \cdot L} = F$~~

$\square \cdot \frac{2\omega \cdot h^2}{3 \cdot L} = F$

Quiz #1

6.



$F = 250\,kN$, $\varepsilon = 0.015$

$\sigma = E\varepsilon$

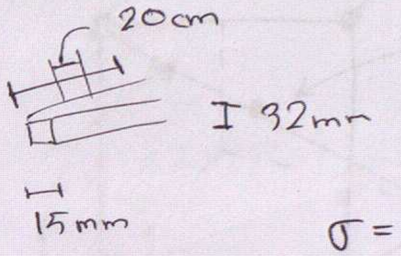
$\frac{F}{A_0} = E\varepsilon \Rightarrow \frac{F}{A_0} \div \varepsilon = E$

$E = \frac{250 \times 10^3\,N}{\pi (17 \times 10^{-3}\,m)^2} \div 0.015 = 1.84 \times 10^{10}\,Pa$

$\approx 18.36\,GPa$

$\approx 18\,GPa$

7.



$E = 50\,GPa = 50 \times 10^9\,Pa$, $F = 90 \times 10^3\,N$

$\sigma = \frac{F}{A_0} = \frac{90 \times 10^3\,N}{(32 \times 10^{-3})(15 \times 10^{-3})(20 \times 10^{-2})} = 937500000$

937.5 MPa

$937.5 \times 10^6\,Pa$

$\varepsilon = \frac{\Delta l}{l_0}$ $\sigma = E\varepsilon$

?

$l_f = l_0 + \Delta l$

$\frac{F}{A_0} = \frac{E \Delta l}{l_0}$

$\Delta l = \frac{F l_0}{A_0 E} = \frac{(90 \times 10^3\,N)(40 \times 10^{-2}\,m)}{[(32 \times 10^{-3})(15 \times 10^{-3})(20 \times 10^{-2})](50 \times 10^9)} = \cancel{75\,m}$

$= 7.5 \times 10^{-3}\,m$

$= 0.0075\,m$

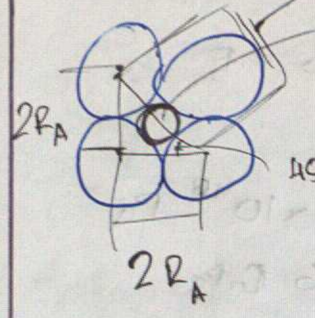
$\Delta l = 0.75\,cm$

$l_f = 40\,cm + 0.75\,cm = 40.75\,cm$

Octahedral Site

$2R_A + 2R_c$

size of cation that perfectly fits



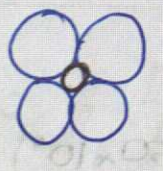
$\frac{R_c}{R_A} \approx$ close to 50% but less

$$\sin 45° = \frac{2R_A}{2R_A + 2R_c}$$

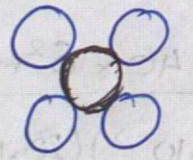
$$\frac{R_A \sin 45°}{R_A} + \frac{R_c \sin 45°}{R_A} = \frac{R_A}{R_A}$$

$$\frac{R_c}{R_A} = \frac{1 - \sin 45°}{\sin 45°} = 0.414 \,//$$

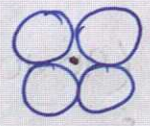
Octahedral



okay ✓



okay ✓



not occurring X

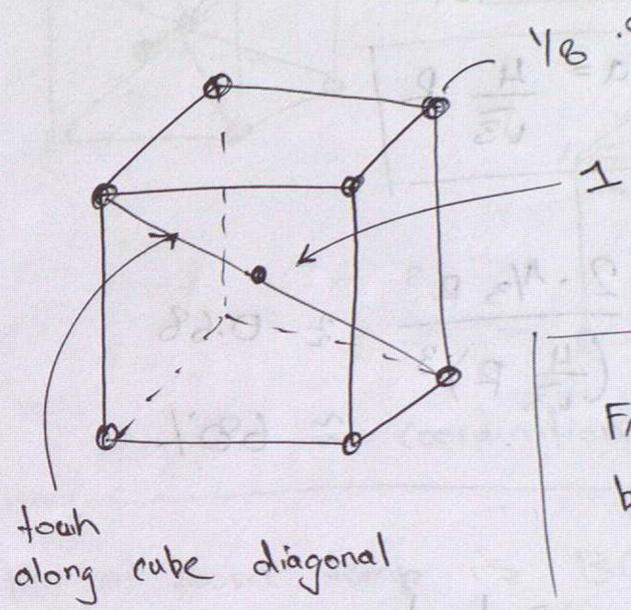
"high energy" or unstable

+ The cation (+) has to be at least ≈41% the radius of the anion (−) to occupy the octahedral interstitial site.

Another metallic structure

Body - centered Cubic (BCC)

ex Fe



touch along cube diagonal

$BCC_{atoms} = 2$

$n_{BCC} = 2$

Fraction of volume occupied by atoms = Atomic Packing Factor (APF)

$$APF_{FCC} \overset{?}{=} \frac{\text{Vol. atoms}}{\text{Vol. unit cell}}$$

ⓘ $a = 2\sqrt{2}R$

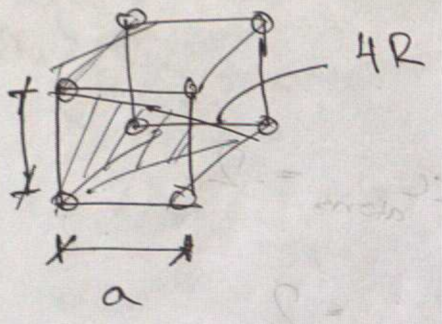
$$= \frac{4 \cdot \frac{4}{3}\pi r^3}{a^3}$$

$$APF_{FCC} = \frac{16\pi r^3}{3(2\sqrt{2}r)^3}$$

$$= \frac{16\pi \cancel{R^3}}{3 \cdot (2\sqrt{2})^3 \cancel{R^3}} \approx 0.74 \approx 74\%$$

BCC - lec 8

Atomic Packing Factor for BCC



$$a_x^2 + a_y^2 + a_z^2 = (4R)^2$$

$$3a^2 = 16R^2$$

$$\boxed{a = \frac{4}{\sqrt{3}} R}$$

$$APF_{BCC} = \frac{2 \cdot 4/3 \pi R^3}{a^3} = \frac{2 \cdot 4/3 R^3}{\left(\frac{4}{\sqrt{3}} R\right)^3} \simeq 0.68$$

$$\simeq 68\%$$

Q.5.2.1

$$\rho = \frac{n \cdot A}{V_c N_A}$$

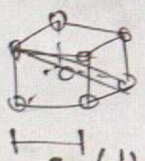
$n_{BCC} = 2$

$A_{Fe} = 55.845\ g/mol$

$R = 124 \times 10^{-12} m$

$N_A = 6.023 \times 10^{23}\ \#/mol$

$$V_c = \left(\frac{4}{\sqrt{3}} R\right)^3$$



$$a^3 = \left(\frac{4}{\sqrt{3}} R\right)^3$$

$$\rho = \frac{2(55.845\ g/mol)}{\left(\frac{4}{\sqrt{3}}(124 \times 10^{-12} m)\right)^3 (6.023 \times 10^{23} \#/mol)}$$

$$= 7896566 \frac{g}{m^3} \times \left(\frac{1m}{100cm}\right)^3$$

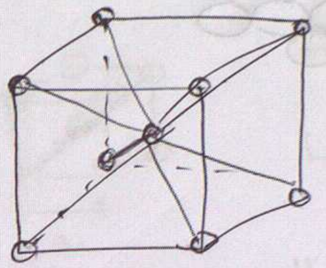
$$= 7.897\ g/cm^3$$

$$\boxed{\simeq 7.9\ g/cm^3}$$

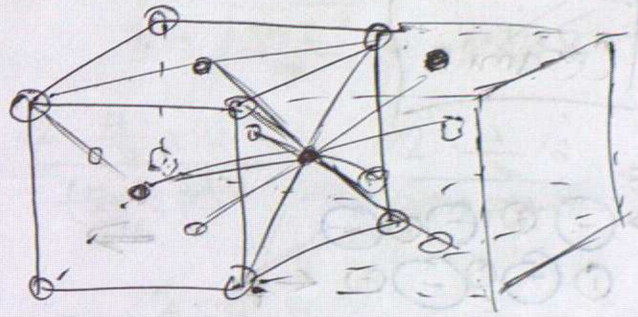
FCC Coordination # - lec 9

BCC

coordination $number_{BCC} = 8$

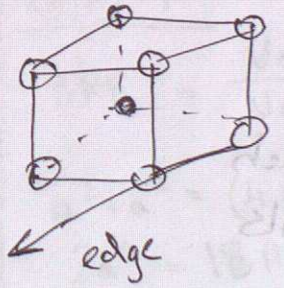


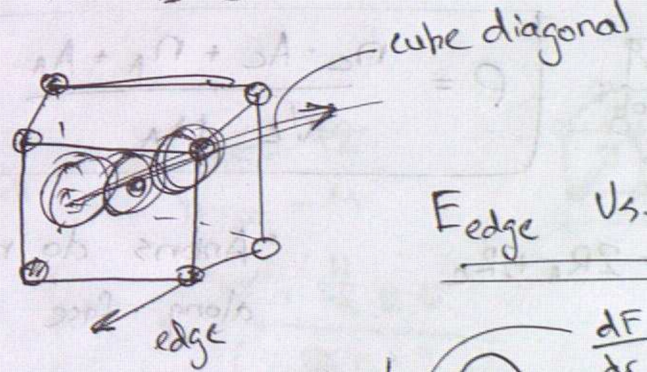
FCC



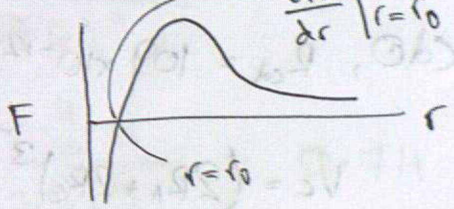
coordination $number_{FCC} = 12$

Fe at room temp is BCC





E_{edge} Vs. $E_{diagonal}$?



$$\left.\frac{dF}{dr}\right|_{r=r_0} \propto E$$

$E_{diagonal}$ = 272 GPa

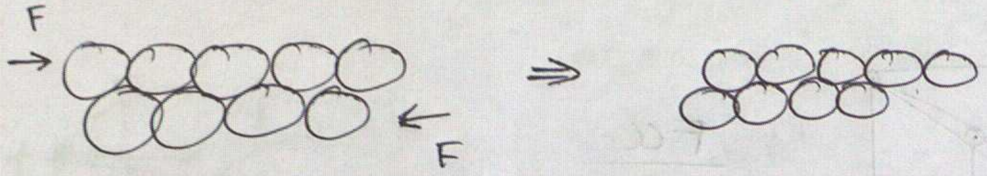
Edge = 125 GPa

- atoms touching along diagonal, so r = less
- atoms at edge have higher r, so $\frac{dF}{dr}$ decreases

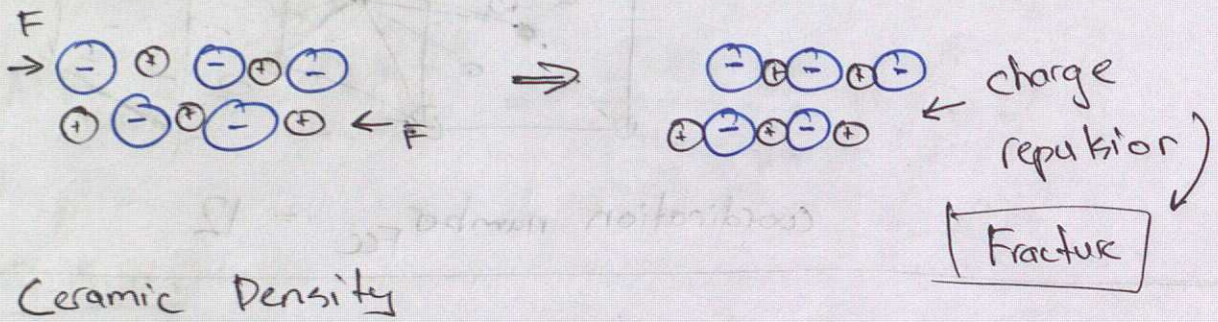
lecture 9

Kitchen sink ✓

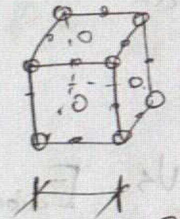
Metal



Ceramic



Ceramic Density



$$\boxed{\rho = \frac{n_c \cdot A_c + n_A + A_A}{V_c \cdot N_A}}$$

$a = 2R_A + 2R_c$

- Anions do not touch along face diagonals

Q.5.1.3 CdO, $R_{cd} = 109 \times 10^{-12}\,m$, $R_o = 126 \times 10^{-12}\,m$

$$V_c = (2R_A + 2R_c)^3 = (2(R_A + R_c))^3$$

$$\rho = \frac{n_{cd} \cdot A_{cd} + n_o + A_o}{(2(R_{cd} + R_o))^3 (N_A)}$$

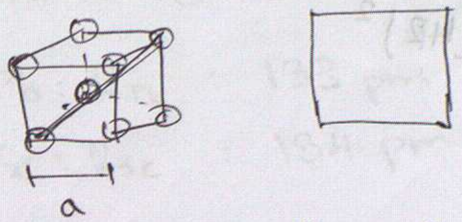
$$= \frac{4(112.41) + 4(15.999)}{(2((109 \times 10^{-12}) + (126 \times 10^{-12})))^3 (6.023 \times 10^{23})} \; [=] \; \frac{g}{m^3}$$

$$= 8213892 \frac{g}{m^3} \cdot \left(\frac{1m}{100cm}\right)^3 = \boxed{8.2\ g/cm^3}$$

5 - Structures

Q.5.4.1

He balloons in BCC, $A_{volume} = 6000\,m^3$, $n_{BCC} = 2$



$$a^2 + a^2 + a^2 = (4R)^2$$

$$3a^2 = 16R^2$$

$$a = \sqrt{\frac{16R^2}{3}} = \cancel{2\sqrt{2}R}$$

$$\frac{V_{atoms}}{V_{cube}} = \frac{n \cdot \frac{4}{3}\pi R^3}{a^3} = \frac{2 \cdot \frac{4}{3}\pi R^3}{\cancel{(2\sqrt{2}R)^3}} = \frac{2 \cdot \frac{4}{3}\pi}{\cancel{(2\sqrt{2})^3}} \approx$$

$$\approx \frac{2 \cdot \frac{4}{3}\pi R^3}{\left(\sqrt{\frac{16R^2}{3}}\right)^3} = \frac{2 \cdot \frac{4}{3}\pi}{\left(\sqrt{\frac{16}{3}}\right)^3} = 0.68 \approx 68\%$$

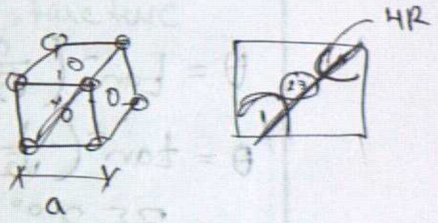
$$\frac{68}{100} = \frac{?}{6000m^3} \quad ? = 4080 \; \{ \; 6000 - 4080 = 1920\,m^3$$

Q.5.9.1

$$APF = \frac{V_{atoms}}{V_{cube/unitcell}}$$

~~$n_{FCC} = 12$~~

$n_{FCC} = 4$



$$a^2 + a^2 = (4R)^2$$

$$2a^2 = 18R^2$$

$$a = \sqrt{\frac{16}{2}R^2}$$

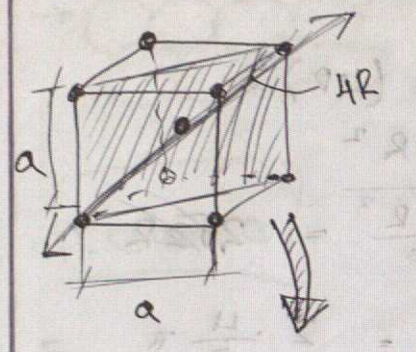
$$= 2\sqrt{2}R$$

$$APF = \frac{\overset{4}{\cancel{12}} \times \frac{4}{3}\pi R^3}{(2\sqrt{2}R)^3}$$

$$= \frac{\overset{4}{\cancel{12}} \times \frac{4}{3}\pi}{(2\sqrt{2})^3} = 0.74$$

Simple Cubic Interstitial Site

$\frac{R_c}{R_A}$ = ? greater than 50%

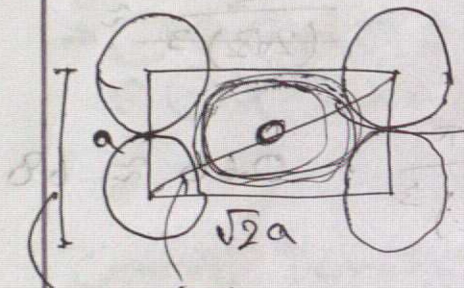


$a^2+a^2+a^2 = (4R)^2$

$3a^2 = 16R^2$

$a\sqrt{3} = 4R$

$a = \frac{4}{\sqrt{3}} R$



~~4~~ $2R_A + 2R_C$ ~~$(a)^2 + (\sqrt{2}a)^2 =$~~

$\sin\theta = \frac{2R_A}{2R_A+2R_C}$

$\frac{\cancel{R_A}\sin\theta}{\cancel{R_A}} + \frac{R_c \sin\theta}{R_A} = \frac{\cancel{R_A}}{\cancel{R_A}}$

$\theta = \tan^{-1}\left(\frac{a}{\sqrt{2}a}\right)$

$\theta = \tan^{-1}\left(\frac{1}{\sqrt{2}}\right)$

$= 35.3°$

$\sin\theta + \frac{R_c}{R_A}\sin\theta = 1$

$\frac{R_c}{R_A} = \frac{1-\sin\theta}{\sin\theta}$

$\frac{R_c}{R_a} = \frac{1-\sin 35.3}{\sin 35.3} \approx 0.732$

$\boxed{\approx 73.2\%}$

---

ex PbSe

semiconductor → crystal structure ?

look at ① stoichiometry , ⓘⓘ radius

Pb : R_{Pb} : 133 pm (cation)

Se : R_{Se} : 184 pm (Anion)

$\frac{R_c}{R_A} = \frac{R_{Pb}}{R_{Se}} = 0.72$

CN = 6

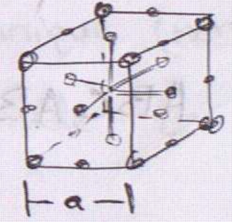
$\frac{R_c}{R_A} = 0.414$

(octahedral interstitial site)

* compare to simple cubic interstitial site

∴ so, $\frac{R_c}{R_A}$ between 0.414 and 0.732 ⟹ octahedral site

so, PbSe is has rock salt crystal structure



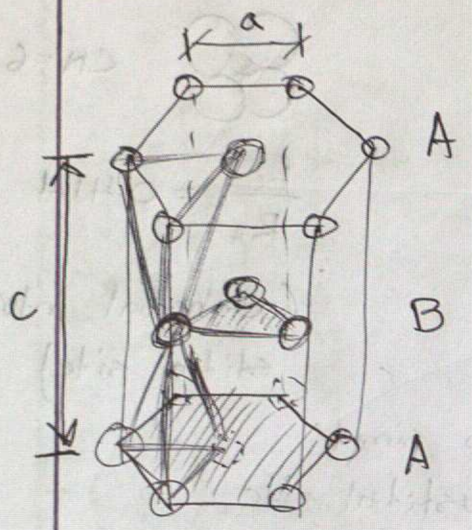
2Ra + 2Rc

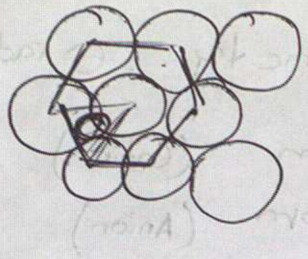
CN = 6 , octahedral interstitial site

Rock Salt Structure

$\rho = \frac{4 \cdot A_{Se} + 4 \cdot A_{Pb}}{(2R_{Se} + 2R_{Pb})^3 \cdot N_A} = 7.5 \text{ g/cm}^3$

Hexagonal Close-Packed (HPC) → same APF as FCC





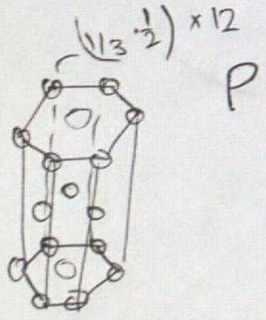
→ HCP is formed from an ABABAB stacking sequence of close-packed planes.

→ FCC is formed from ABCABC

Q.5.6-1

Co, HCP, $A = 58.933$ g/mol, $R = 135\times10^{-12}$ m

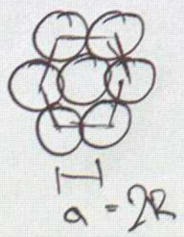
$c = 1.633a$, $V = \frac{3\sqrt{3}}{2}a^2c$



$$P = \frac{n\cdot A}{V_c\cdot N_A} = \text{density}$$

$$V_c = \frac{3\sqrt{3}a^2c}{2}$$

$$n_{HCP} = \left(\frac{1}{3}\cdot\frac{1}{2}\right)\times12+3+1$$
$$= 6$$



$a = 2R$

$c = 1.633(2R)$

$c = 3.266R$

Q.5.6.1

$$P = \frac{n\cdot A}{V_c\cdot N_A}$$

$$= \frac{6\,(58.933\ \text{g/mol})}{\left(\frac{3\sqrt{3}}{2}\left(2(135\times10^{-12}\text{m})\right)^2\left(3.266(135\times10^{-12}\text{m})\right)\right)\left(6.023\times10^{23}\ \frac{\#}{\text{mol}}\right)}$$

$$= 7030198\ \text{g/m}^3\cdot\left(\frac{1\text{m}}{100\text{cm}}\right)^3$$

$$= 7.03\ \text{g/cm}^3$$

Notes from Ch.5

- FCC has 4 unique (non-parallel) close-packed planes
- Al pop cans made bc. Al has FCC (easy to mould)

APF of HCP

$$\frac{V_{atoms}}{V_{unit\ cell}} = \frac{n\cdot\frac{4}{3}R^3}{\left(\frac{3\sqrt{3}}{2}a^2\right)h}$$

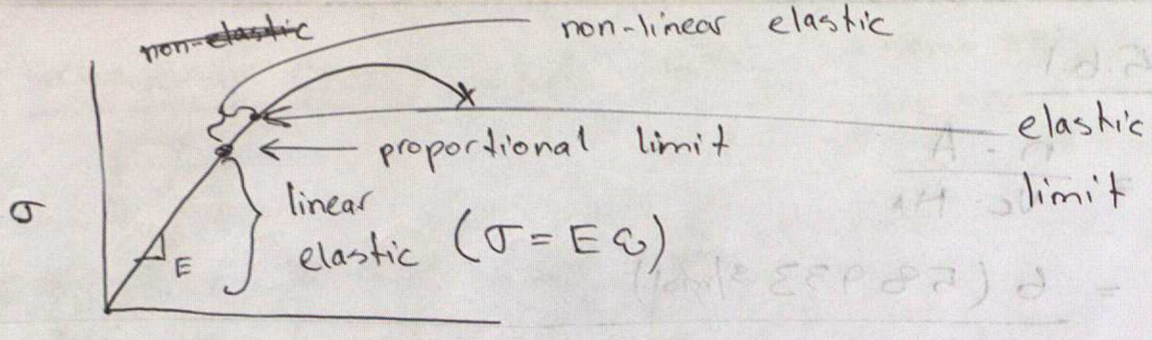
$a = 2R$ — $a^2 = (2R)^2 = 4R^2$

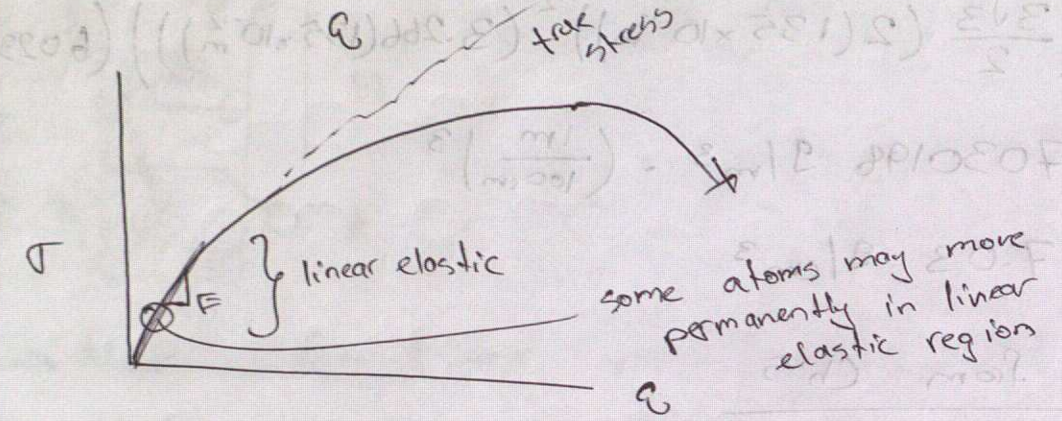
$h = 2a\sqrt{\frac{2}{3}}$

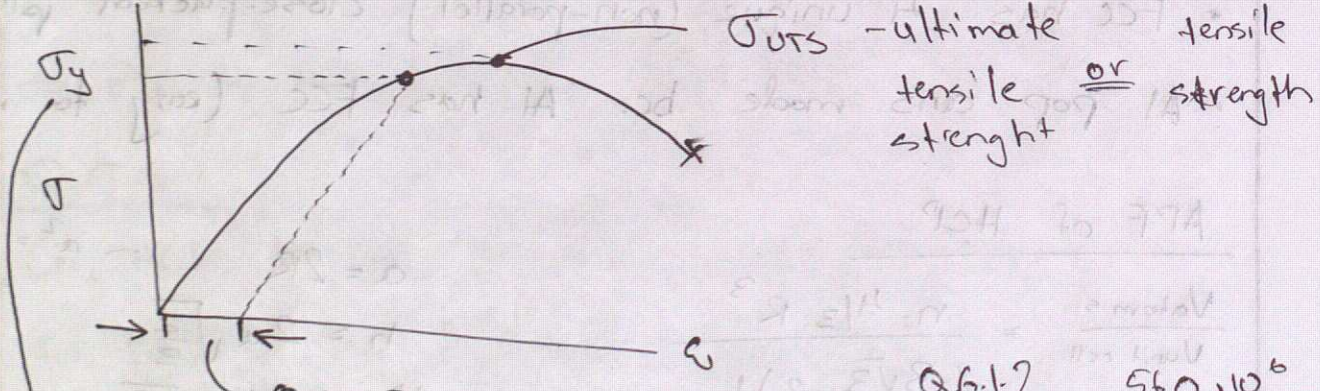
$h = 4R\sqrt{\frac{2}{3}}$

$h = 3.266R$

Lecture 11







0.002

ε = 0.002

or 0.2%

yield strength (σ_y)

in practice, we say elastic until yield strength

" 0.2% offest yield strength "
offset

$\sigma = E\varepsilon$
$= (200\times10^9)(0.002)$
$= 4\times10^8 Pa$

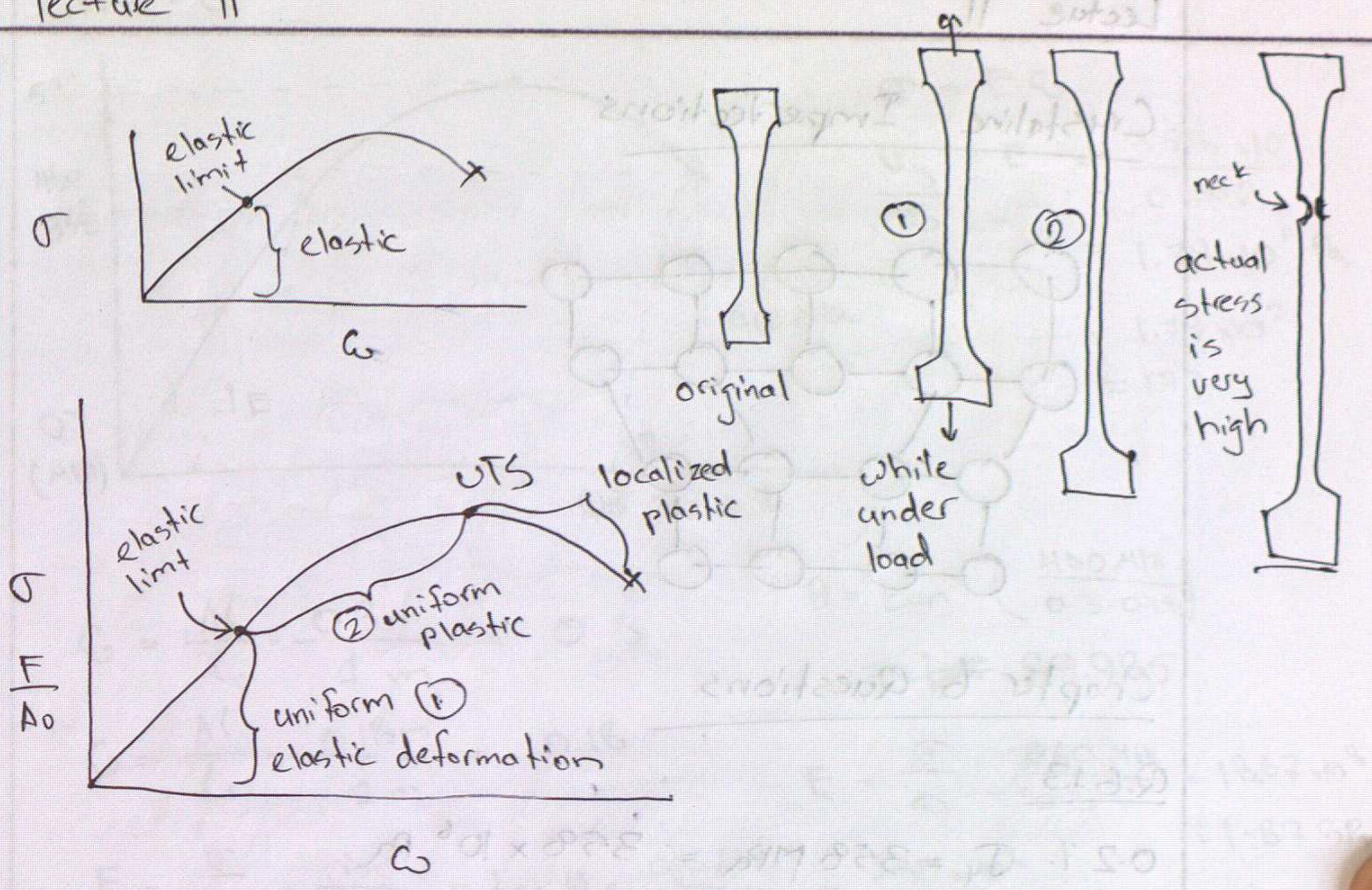
Q.6.1.2

$\sigma_y = \frac{F}{A_0}$

$F = \sigma_y A_0$
$= (560\times10^6)(100\times10^{-3})$
$= (4\times10^8 Pa)(100\times10^{-3} m)^2$
$= 4$

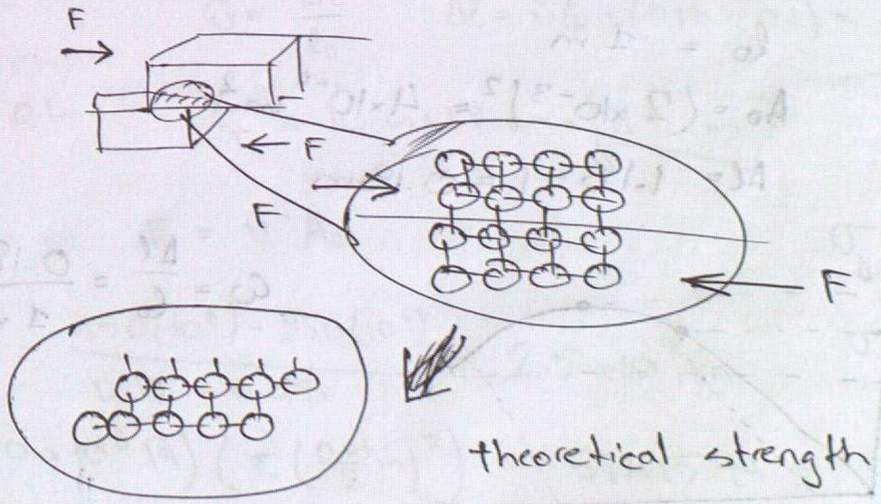
$\frac{560\times10^6}{0.002} =$

lecture 11



Plastic Deformation at Atomic Level

Imagine a single crystal



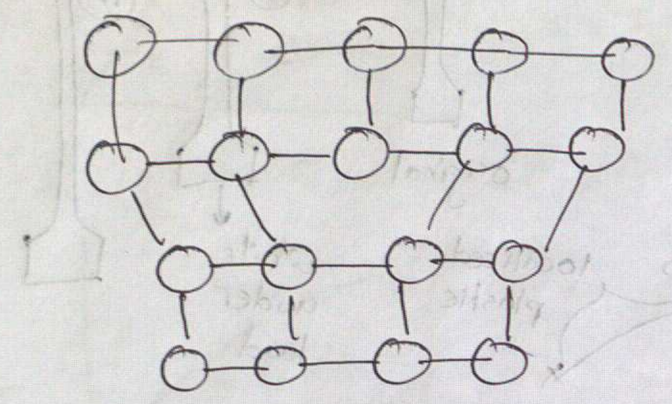
not entirely correct

theoretical strength is 5 X more than experimental

"Problem"

Lecture 11

Crystaline Imperfections



Chapter 6 Questions

Q.6.1.3

0.2 % $\sigma_y = 358 \text{ MPa} = 358 \times 10^6$ Pa

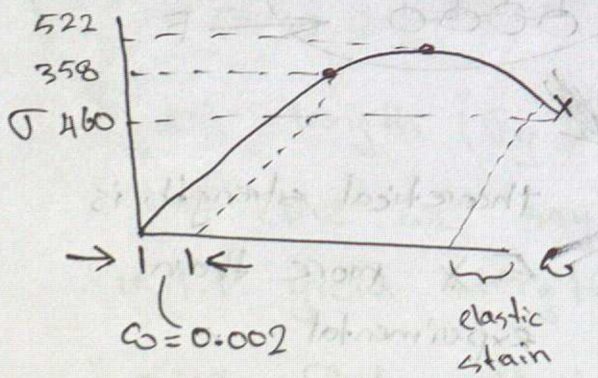
UTS = 522 MPa = 522×10^6 Pa

$\sigma_{fracture} = 460 \times 10^6$ Pa

$l_0 = 1$ m

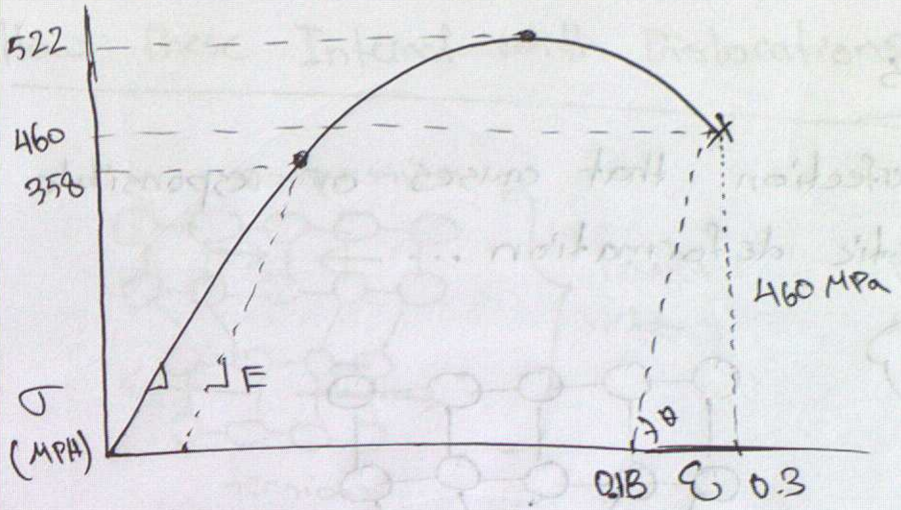
$A_0 = (2 \times 10^{-3})^2 = 4 \times 10^{-6}$ m^2

$\Delta l = 1.18 - 1 = 0.18$m



$\varepsilon = \frac{\Delta l}{l_0} = \frac{0.18\text{m}}{1\text{ m}} = 0.18$

Ch.6 - Q



$\sigma = E\varepsilon$

$\frac{\sigma_y}{\varepsilon} = E = \frac{358 \times 10^6}{0.002}$

$= 1.79 \times 10^{11}$ Pa

$= 1.79 \times 10^2$

≈ 179

$\theta = \tan^{-}\left(\frac{460 \text{ MPA}}{0.3 - 0.18}\right)$

$=$ ~~15~~ 89.985

$\varepsilon = \frac{\Delta l}{l_0} = \frac{0.3\text{m}}{1\text{ m}} = 0.3$

$\varepsilon = \frac{\Delta l}{l_0} = \frac{0.18\text{m}}{1\text{ m}} = 0.18$

$E = \frac{\sigma}{\varepsilon} = \frac{460 \text{ MPa}}{0.3} = 18.67 \times 10^8$

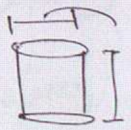
≈ 1.87 GPa

$E = \frac{\sigma}{\varepsilon} = \frac{\text{rise}}{\text{run}} = \tan\theta = \frac{\text{opp (rise)}}{\text{adj (run)}} = \frac{460 \times 10^6}{0.12} = 3.83 \times 10^9$ Pa

$\boxed{= 3.83 \text{ GPa}}$

Q.6.5.1a/b

a)



$\varepsilon = \frac{\Delta l}{l_0}$ $\Delta l = \varepsilon l_0 = (0.18)(0.1) = 0.018$ m

$= 1.8$ cm

$l_T = 10\text{cm} + 1.8 \text{ cm} = \boxed{11.8 \text{ cm}}$

b) $\sigma = \frac{F}{A_0} \Rightarrow F = \sigma A_0$

$\sigma_{UTS} = 400$ MPa

$E = \frac{\sigma}{\varepsilon} = \frac{350(10^6) - 250(10^6)}{0.12 - 0.08} = 2.5 \times 10^9$ Pa

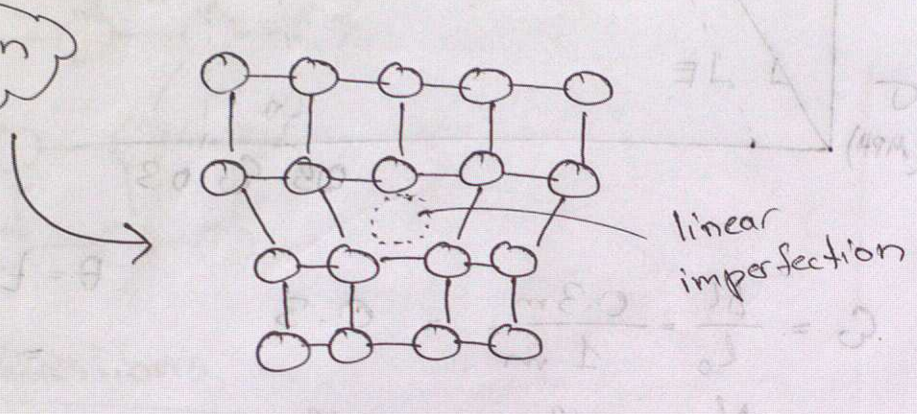
$\sigma = \frac{F}{A_0} \Rightarrow$

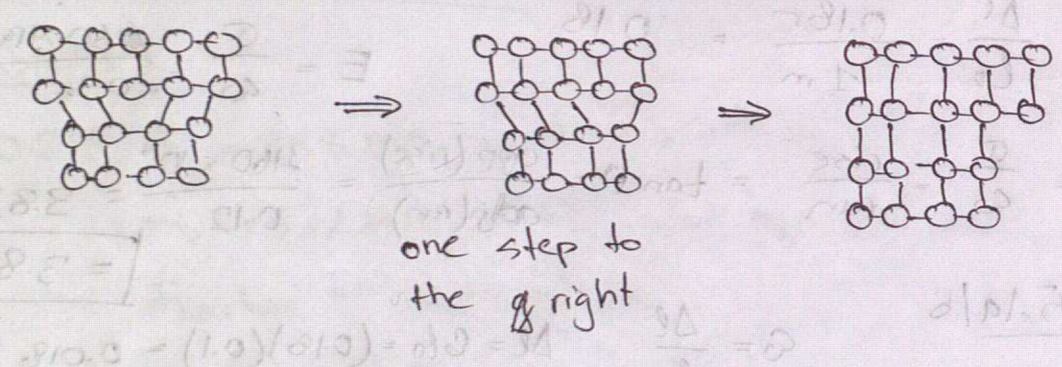
$F = (400 \times 10^6 \text{ Pa})\left(\pi\left(\frac{0.01}{2}\text{m}\right)^2\right) = 31415 \text{ N} \approx 31.4 \text{ KM}$

Imperfections

ex The imperfection that causes or responsible for plastic deformation ...

Dislocation

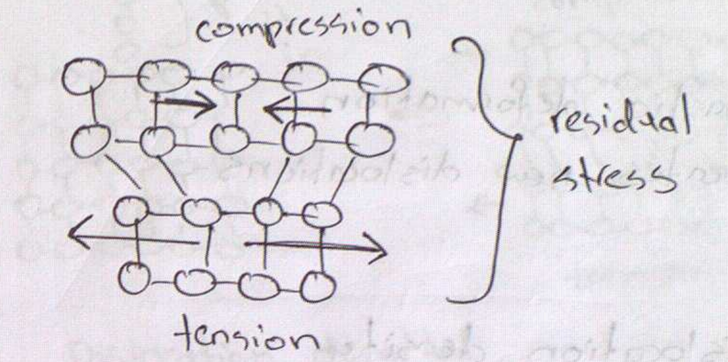


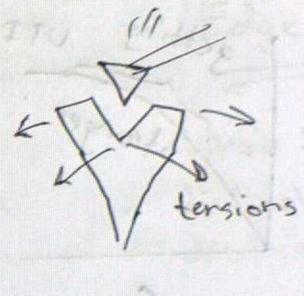


Organizing Imperfections (by dimensionality)

- 0-dimensional (point defects)
- 1-dimensional (linear / dislocation)
- 2-dimensional (interfaces) - grain boundary / free surfaces
- 3-dimensional (second phases) - pores (volume)

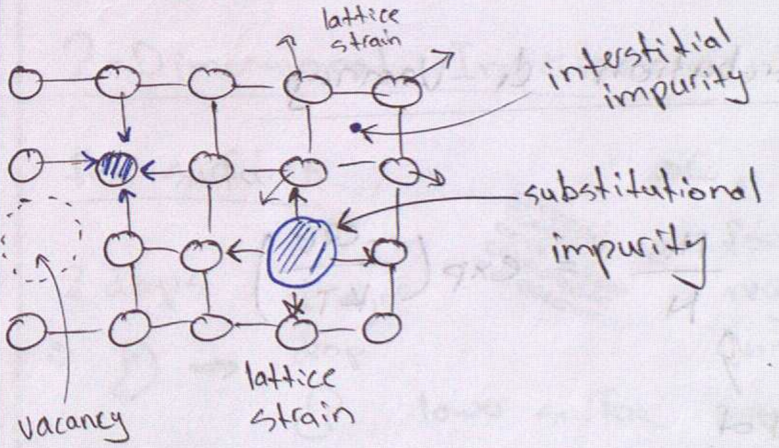
How These Interact With Dislocations





0-Dimensional

1. Impurity in solid solution



dislocations have difficulty moving past impurities } increase in strength

Vacancy

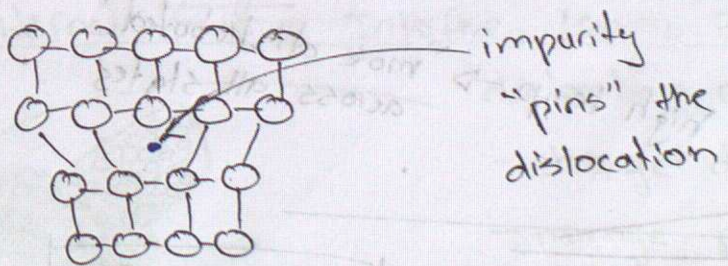
$$\boxed{\frac{N_v}{N} = \exp\left(\frac{-Q_v}{kT}\right)}$$

energy to form vacancy

\# of vacancies

Boltzman constant

temp in K



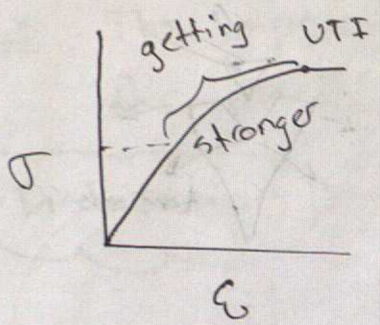
Impurities inhibit impurity movement

↳ impurities strengthen materials

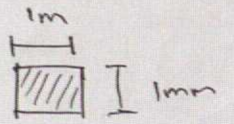
- impurity jumps around, but eventually ends up at dislocation location.
- impurities diffuse towards dislocations

Lecture 12

Strain Hardening



plastic deformation creates new dislocations

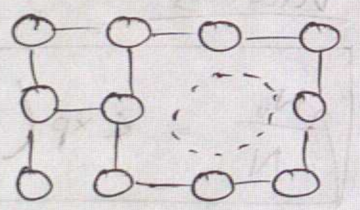


dislocation density

# of dislocations /area

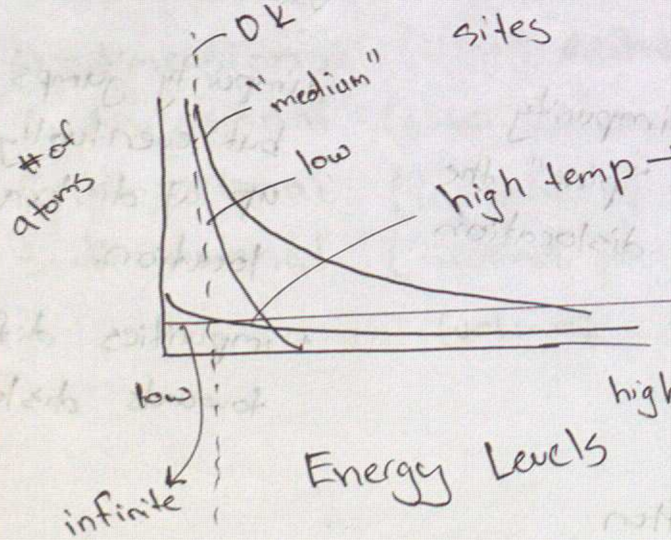
$10^4 - 10^{10}$ dislocations /mm^2

The Boltzman Distribution & Vacancy



$$\frac{N_v}{N} = \exp\left(\frac{-Q_v}{KT}\right)$$

# of sites



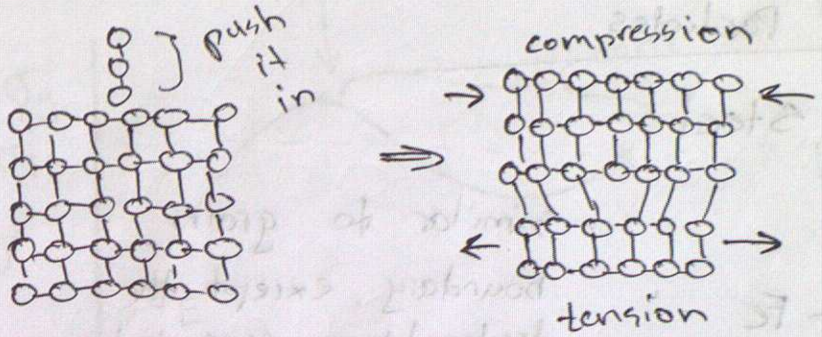
high temp → "more distributed" across all states

$$\boxed{\frac{N_v}{N} = e^{\frac{-Q_v}{KT}}}$$

0 kelvin → only low energy state
"absolute 0"

Ch. 7

1-Dimensional Imperfections (Dislocations)



Edge dislocation

"strain fields" around dislocation inhibit dislocation movement

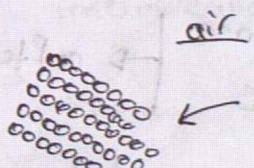
Dislocation density

$10^4/mm^2$ — $10^{10}/mm^2$
annealed — heavily deformed

- cold/warm work
- cold/warm forging
- strain hardening

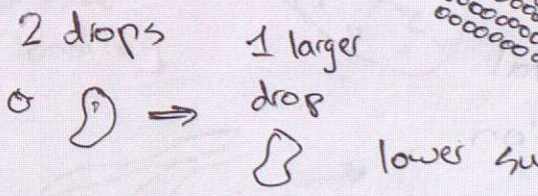
2-Dimensional Imperfections (Interface)

free surfaces



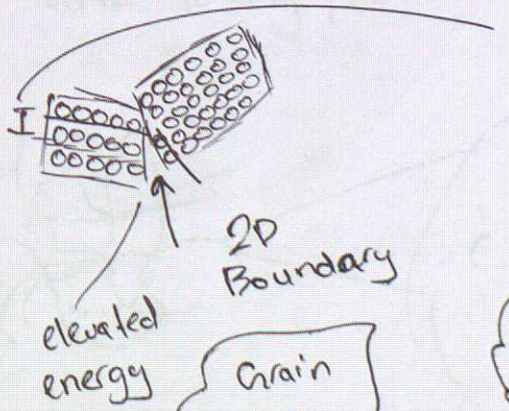
← fewer nearest neighbor atoms (unsatisfied bonds)

"elevated energy"
↓
surface energy



lower surface area/volume
lower surface energy

Internal ~~Surface~~ Interface / Grain Boundaries

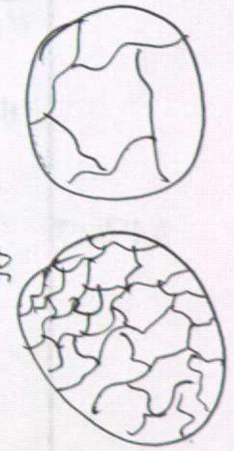


dislocation at grain boundary must:
- change direction
- manage planar mismatch
- lattice strain

Grain boundary inhibits dislocation movement

Grain size reduction

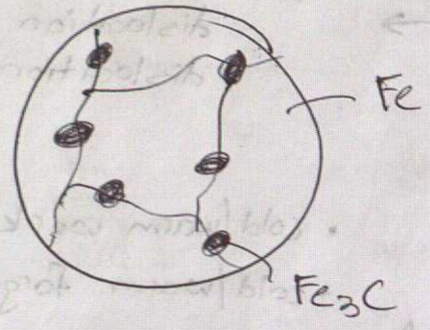
→ Strengthen metal by decreasing grain size



Ch.7 / Lec 13

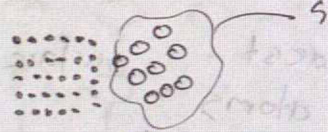
3-Dimensional Imperfections or Second Phase Particles

eg Fe_3C in Steel



- similar to grain boundary, except the dislocation runs into hard, brittle second phase particles instead of another grain

+ pores (bubbles)
+ second phase particles



→ often hard phases

+ material with different crystal structure → 3-D imperfection
+ Eg: AA6061 - T6 Aluminum

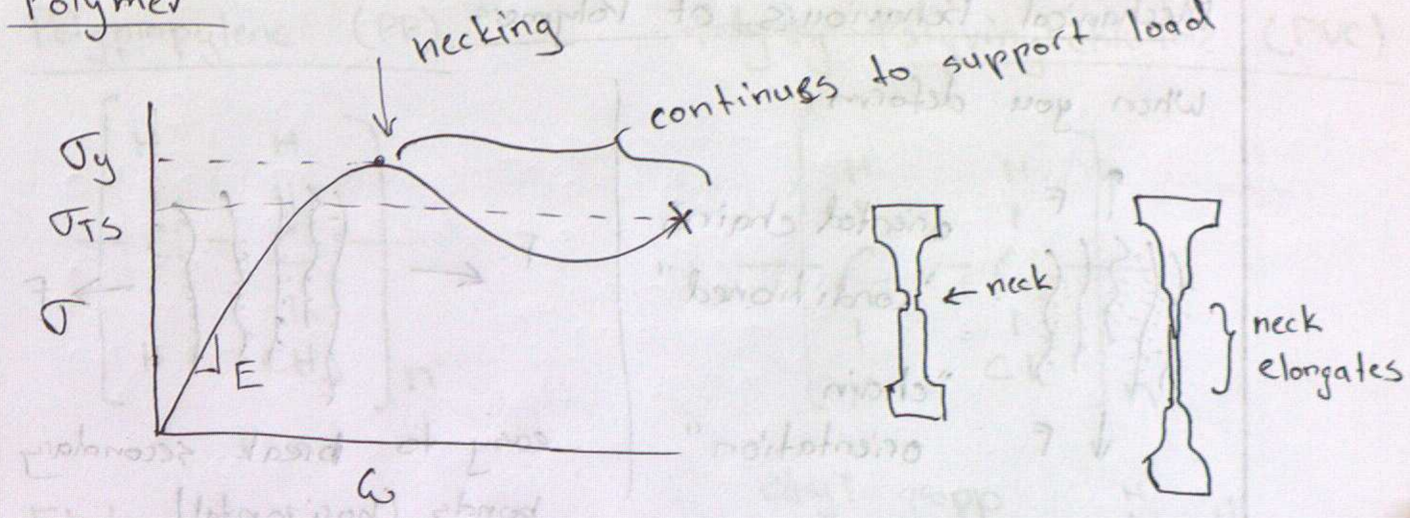
T6 heat treatment

Q.7.13.1

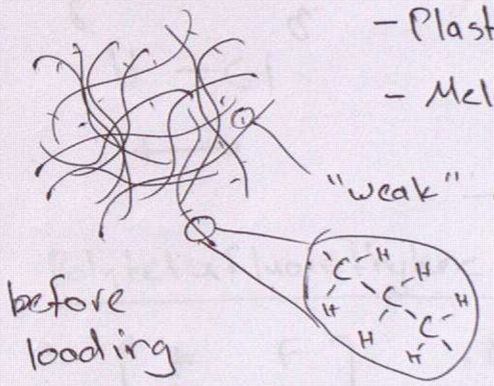
T, T, F, T, F

Ch.8 / Lec 13

Polymer



Polymer Structure

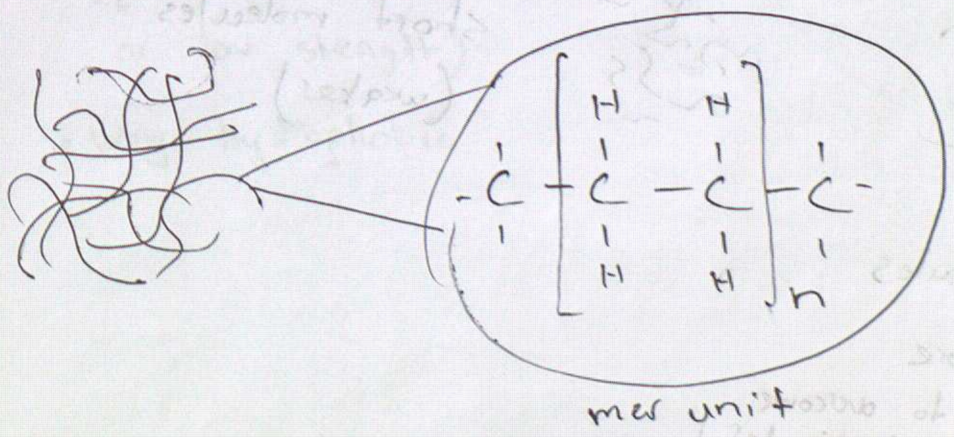


- Plast Deformation → strings slide past ea. other
- Melt → add thermal energy
- Dissolution

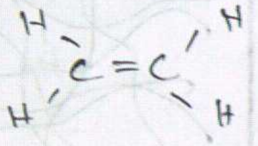
after loading / deformation.

many poly mer — mer unit "building block"

Polyethylene (PE)



$$-C-\left[\begin{matrix} H & & H \\ C & - & C \\ H & & H \end{matrix}\right]_n-C-$$



$H_2C=CH_2$

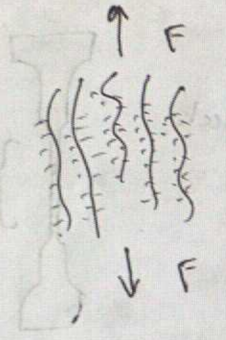
ethylene

"ethene" IUPAC

Ch.8 | Lec 14

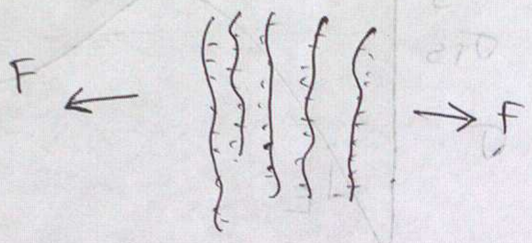
Mechanical Behaviours of Polymers

When you deform



oriented chains
"conditioned"

"chain
orientation"



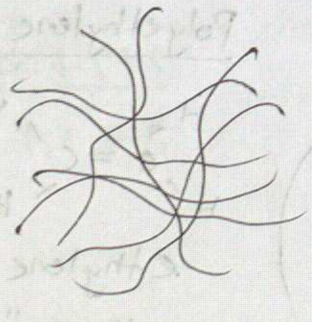
easy to break secondary bonds (horizontal)

- chain orientation to strengthen Specta™ and Dyneema®

How to strengthen Polymer?

1) long molecules (stronger)
short molecules (weaker)

[PE used in orthopeadic applications is UHMWPE → ultra high molecular weight polyethylene]



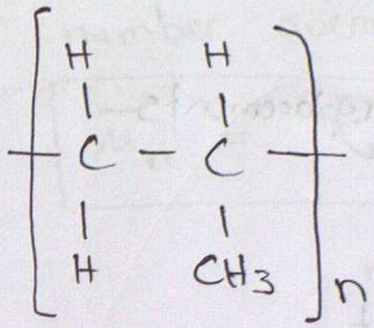
long molecules

(stronger, more secondary bonds to overcome before plastic def.)

short molecules
(weaker)

Ch.8 -Polymers

Polypropylene (PP)

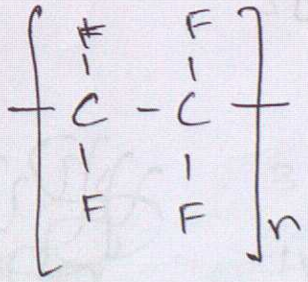


$$\left[-\overset{H}{\underset{H}{C}} - \overset{H}{\underset{CH_3}{C}} - \right]_n$$

Electonegativity

$$\overset{\longleftrightarrow}{\overset{\delta^+}{H} - \overset{\delta^-}{Cl}}$$

Polytetrafluorethylene (PTFE)



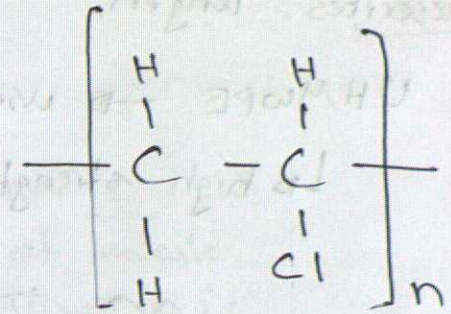
$$\left[-\overset{F}{\underset{F}{C}} - \overset{F}{\underset{F}{C}} - \right]_n$$

- Gore-Tex
- Teflon → ePTFE elongated

(quite mechanically weak or low strength)

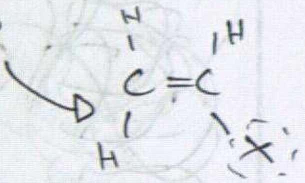
- very hydrophobic

~~Poly vy.~~ Polyvinylchloride (PVC)

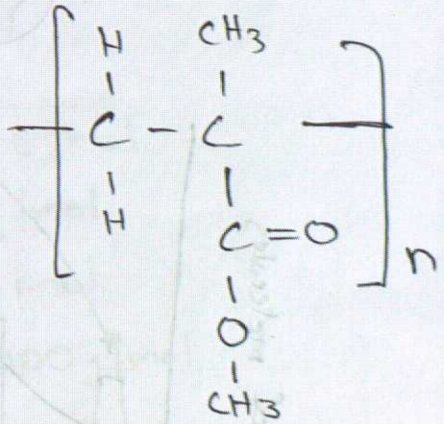


$$\left[-\overset{H}{\underset{H}{C}} - \overset{H}{\underset{Cl}{C}} - \right]_n$$

vinyl group



Polymethylmethacrylate (PMMA)

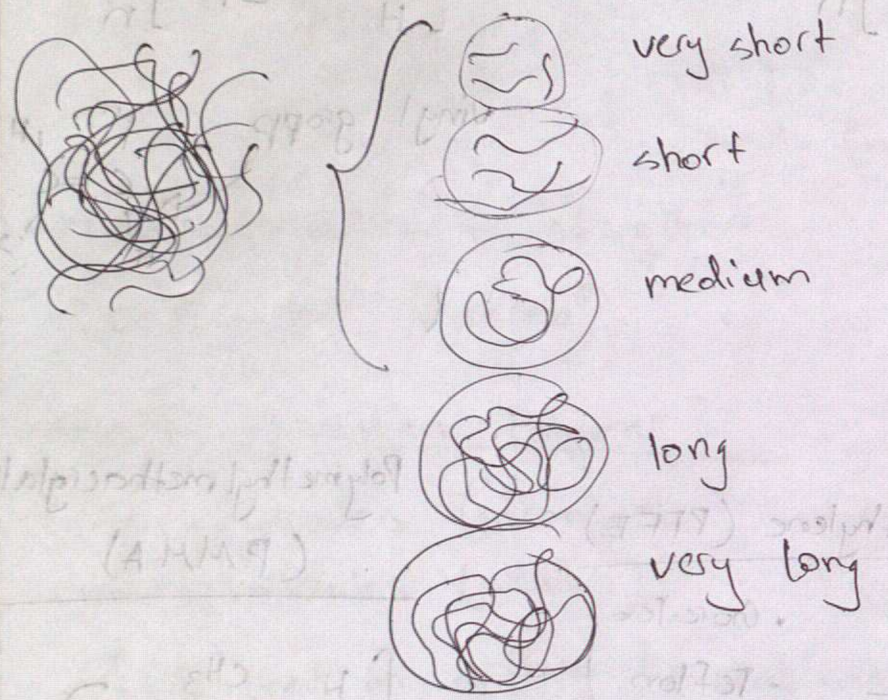


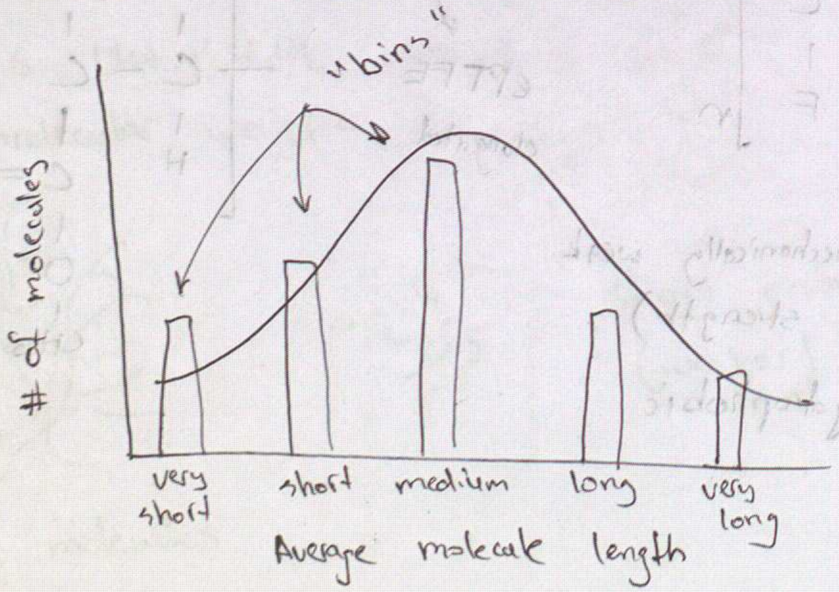
$$\left[-\overset{H}{\underset{H}{C}} - \overset{CH_3}{\underset{\underset{\underset{CH_3}{O}}{C=O}}{C}} - \right]_n$$

Molecular Weight

- describes length.

ex UHMWPE → used in hip replacements
↳ high strength





Calculating Molecular Weigth

① number average M.W

$$\boxed{\overline{M}_n = \sum x_i M_i}$$

average M.W. of molecules in group i

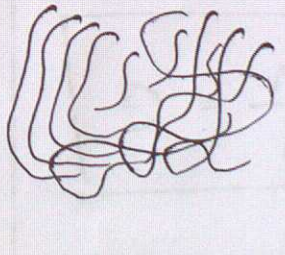
number fraction of group i

② Weight average M.W

$$\boxed{\overline{M}_w = \sum w_i M_i}$$

weigth fraction of group i

ex



3 "short" 5000 g/mol
4 "medium" 8000 g/mol
2 "long" 11000 g/mol
1 "really long" 14000 g/mol

$$\overline{M}_n = \frac{3 \cdot 5000 + 4 \cdot 8000 + 2 \cdot 11000 + 1 \cdot 14000}{10} = 8300$$

$$= \sum x_i M_i = \frac{3}{10} \cdot 500 + \frac{4}{10} \cdot 8000 + \frac{2}{10} \cdot 11000 + \frac{1}{10} \cdot 14000$$

numbers fraction

Lec 15

Molecular Weight

weight fraction

$$\bar{M}_w = \left(\frac{3 \cdot 5000}{3 \cdot 5000 + 4 \cdot 8000 + 2 \cdot 11000 + 1 \cdot 14000}\right) \cdot 5000 +$$

$$\left(\frac{4 \cdot 8000}{3.5k + 4.8k + 2.11k + 1.14k}\right) 8000 \quad \cdots$$

* $\bar{M}_w$ always higher than $\bar{M}_n$

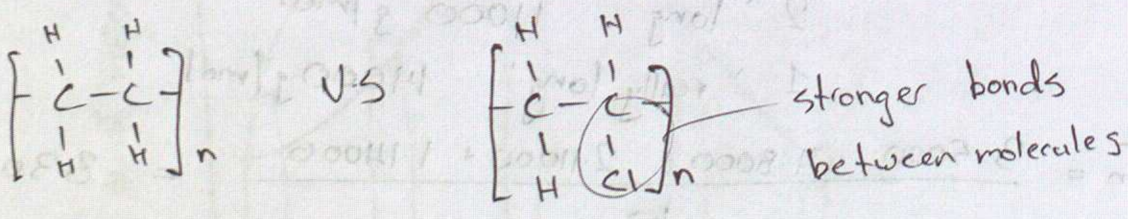
$$\bar{M}_w = \sum w_i M_i = \underbrace{\left(\frac{3 \cdot 500}{total}\right)}_{w_1} \overset{M_1}{5000} + \underbrace{\left(\frac{4 \cdot 800}{total}\right)}_{w_2} \overset{M_2}{8000} + \cdots$$

$= 9265$ g/mol

How to Strengthen Polymer

2) make "weak" bonds between chains stronger

ex



Ch.8

Molecular Weight

$$\boxed{\bar{M}_{number} = \sum_{n=1}^{i} M_n x_n}$$

M_n : molecular weight of n^{th} grp.

x_n : # fraction of n^{th} grp.

$\left(\frac{\text{\# of molecules in that group}}{\text{total \# of molecules}} \right)$

box of candy

10g ×5

50g ×4

100g ×3

$$\bar{M}_n = 10g \cdot \frac{5}{12} + 50g \cdot \frac{4}{12} + 100g \cdot \frac{3}{12}$$

$= 45.8$ g/bar

$$\boxed{\bar{M}_{weight} = \sum_{n=1}^{i} M_n w_n}$$

M_n : molecular weight of n^{th} group

w_n : weight fraction of n^{th} group

$\left(\frac{\text{combined mass of molecu. in that grp.}}{\text{total mass of all molecules}} \right.$

box of candy

10g ×5

50g ×4

100g ×3

$$\bar{M}_w = 10g \cdot \frac{50}{550} + 50 \cdot \frac{200}{550} + 100 \frac{300}{550}$$

$= 73.6$ g/bar

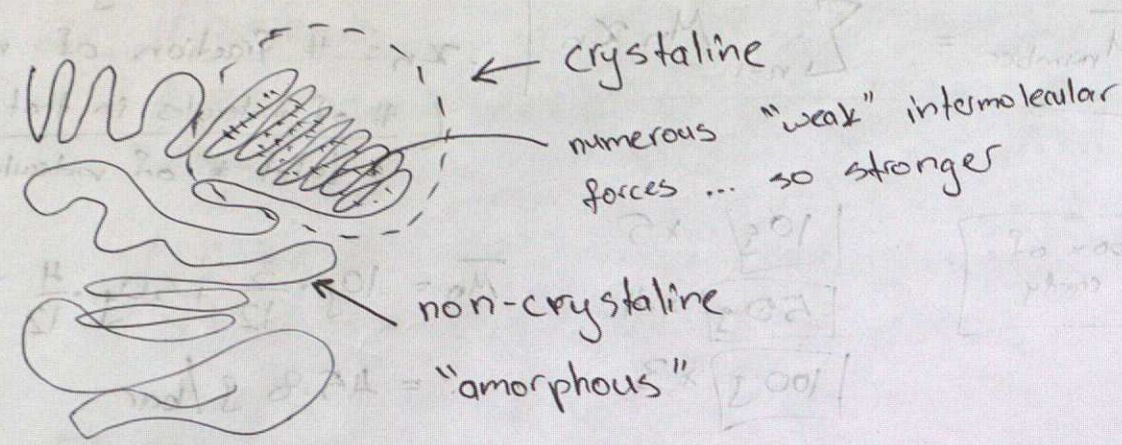
$$\boxed{Đ = \frac{M_{weight}}{M_{number}}}$$

Strengthening Polymers

1) chain length (high molecular weight) ex UHMWPE
2) chain orientation ex Spectra
3) stronger dipoles (intermolecular "weak" forces) ex PVC
4) increase crystalinity

Lec 17

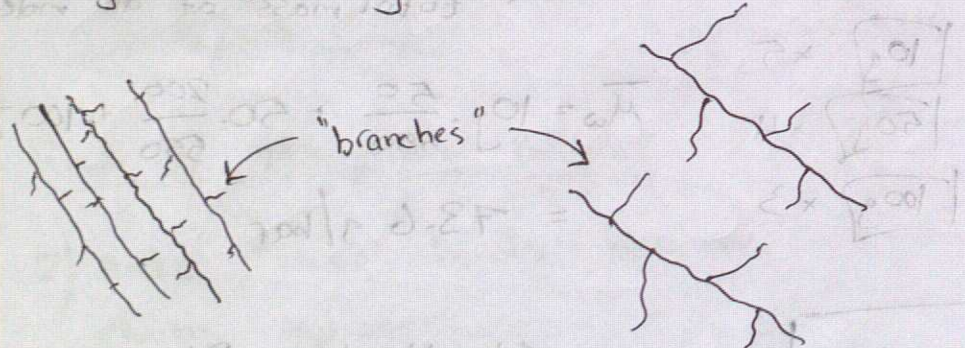
Organizing Molecules



ex HDPE vs. LDPE

- high density
- higher crystalinity

- low density



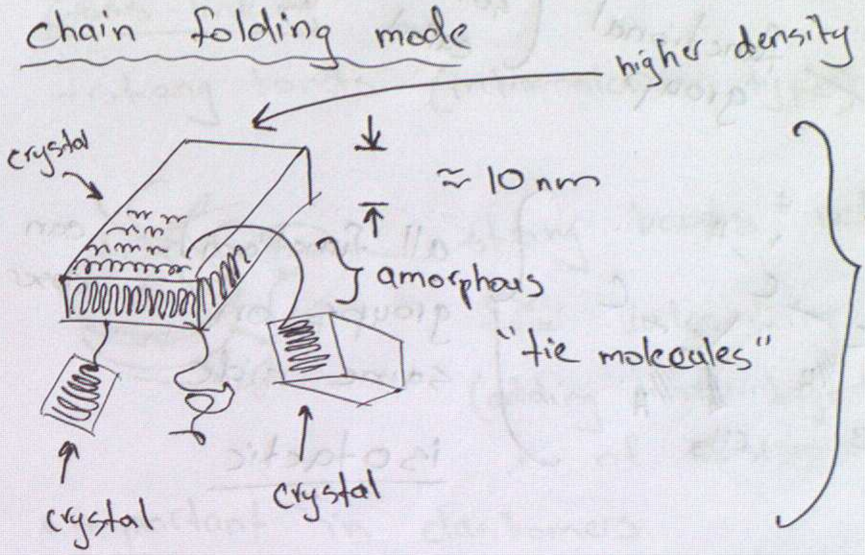
- fewer and smaller branches
- can pack them closer together
- higher σ, E

- softer, easier to dissolve
- molecules can't get as close, so low density and weaker

Lec 18

Models of Crystalinity

Chain folding mode

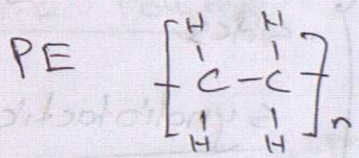


- polymer is never 100% crystaline
- may be completely amorphous

How to encourage Crystalinity

- simple mer units

  ex PE



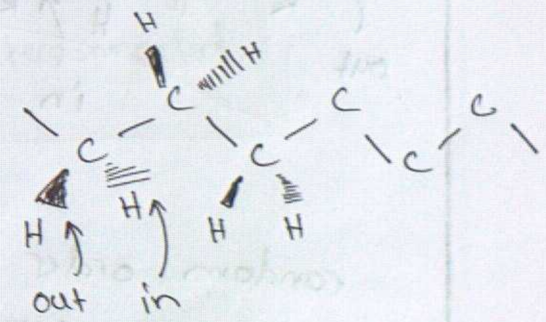
$$\left[\begin{matrix} H & H \\ | & | \\ C - & C \\ | & | \\ H & H \end{matrix} \right]_n$$

- fewer branches

  ex $\boxed{\text{HDPE}}$ ✓ vs. LDPE

- regular repeating structures

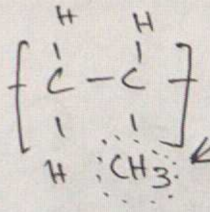
- predictable 3-Dimensional structure



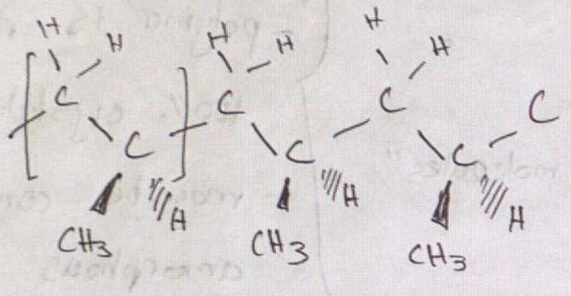
Lec 18

3-D Drawings Tacticity (how arranged in 3-D)

PP

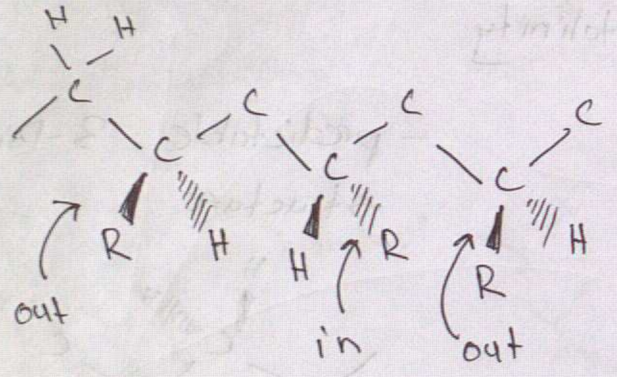


functional group (sometimes called "R")



all functional groups on same side } isotactic

can stack closer together



functional groups on alternating sides } syndiotactic

cannot stack so close

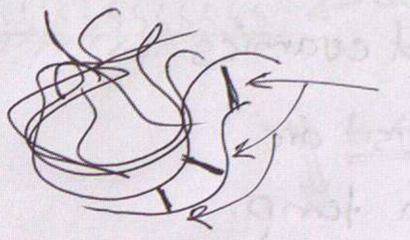
random order of functional sticking in or out } atactic (elastomers, weak, but high strain to failure)

Ch.8

Cross-linking and Network Polymeis

Cross-linking

- strong bonds (intramolecular type) "covalent"



stong bonds between chains

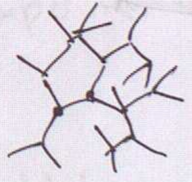
ex Vulcanizing rubber (adding cross-linkage to make stronger)

ex. of elastomer, shoe sole (adding sullfur)

* important in elastomers

ex PEX tubing (residensial water piping, stronger, higher pressure and temperatare)

Network Polymer



3-Dimensional interconnected network

ex Epoxy

- high strength
- little bit brittle

Lec 18

Time and Temperature

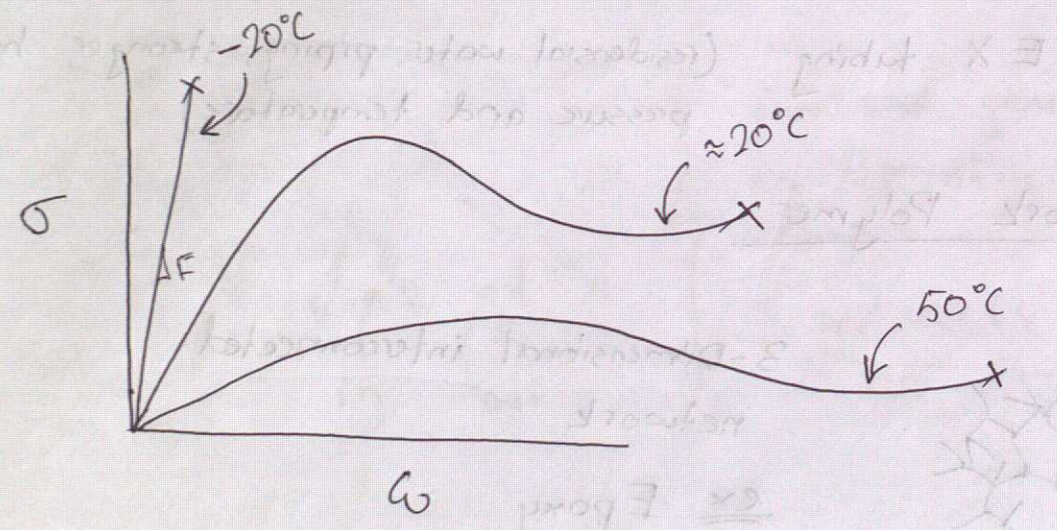
Time ↑ strain rate

Temperature ↑ small changes close to room temperature

ⓘ doesn't matter for metals and ceramics

- intermolecular bonds in polymers are affected by small changes in temp.

<u>ex</u> Plexiglass®

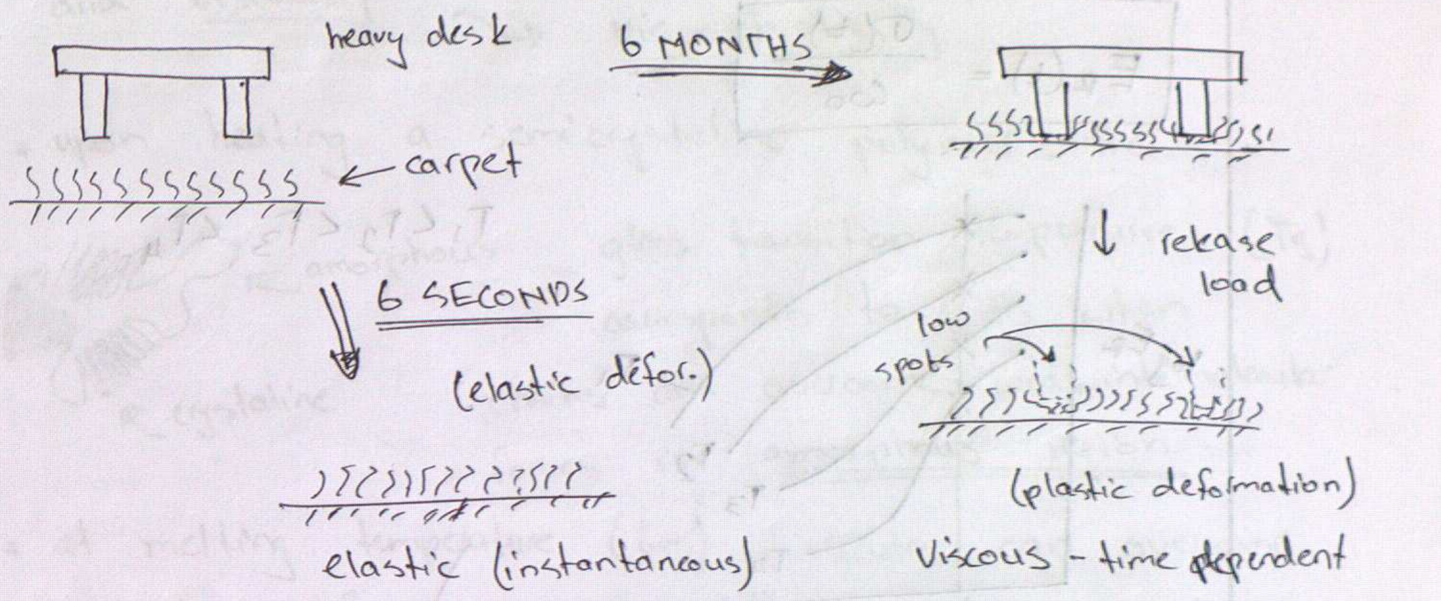


- competition between binding energy and thermal energy.

- polymer low temp → brittle
  high temp → viscous / flowy

Ch. 8 / Lec 19

Polymers and Strain Rate



- Polymers are <u>viscoelastic</u>.

Relaxation Modulus

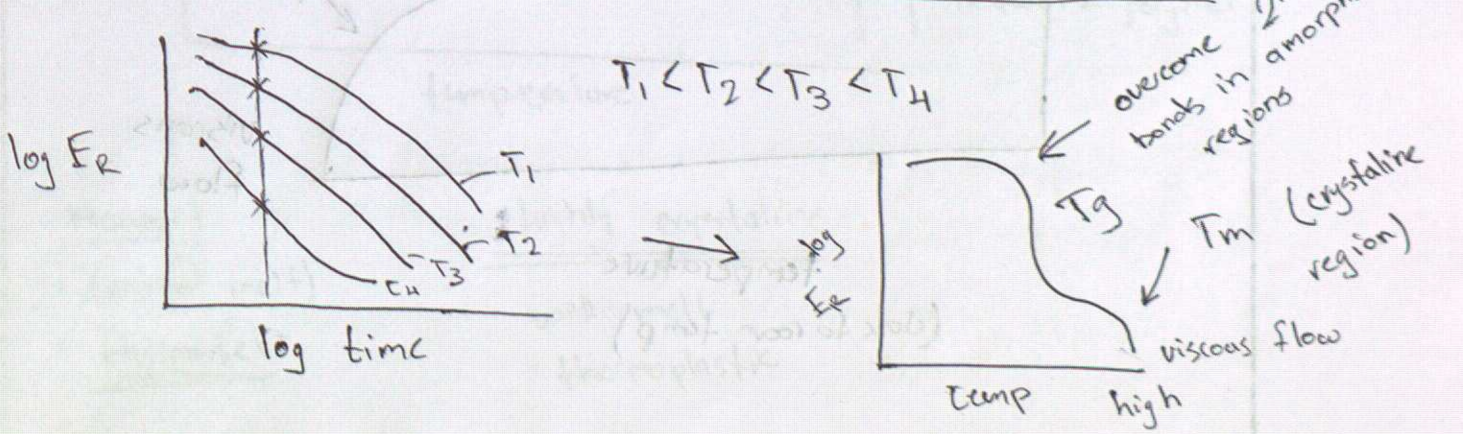
→ load applied σ_0 → observed strain changing

→ Experimentally : apply fixed strain ε_0 → observe stress relaxing with time

<u>ex</u> Nylon strings on guitar

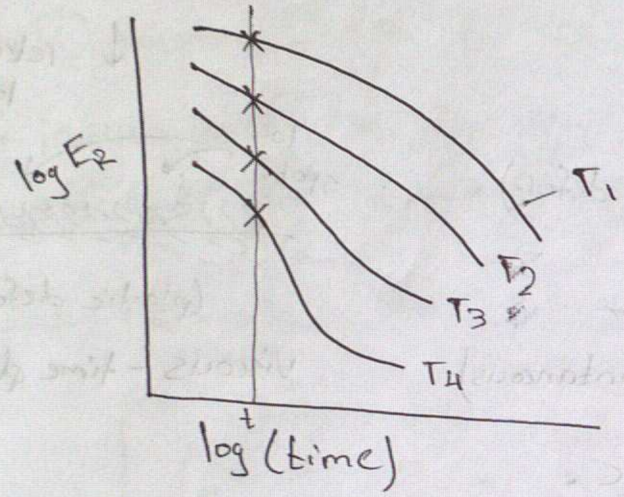
Define <u>Relaxation Modulus</u>

$$\boxed{E_R = \frac{\sigma(t)}{\varepsilon_0}}$$



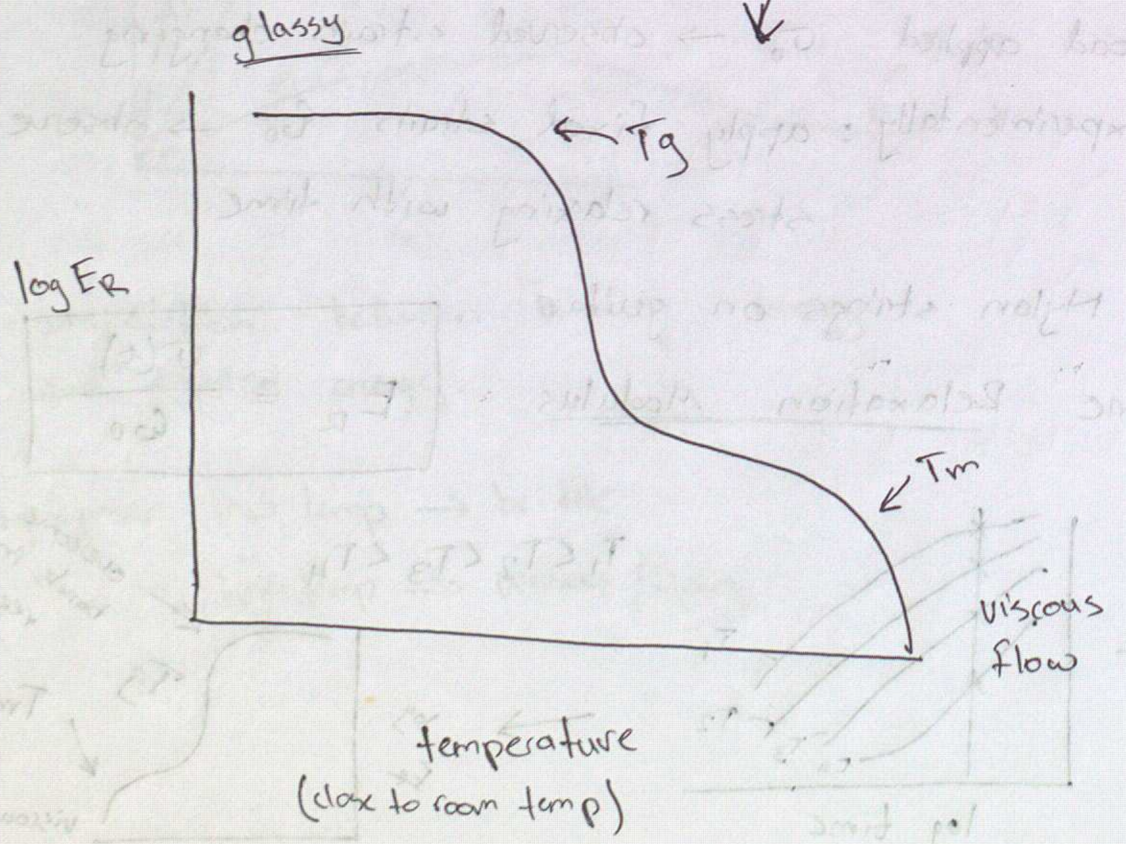
Relaxation Modulus

$$\boxed{E_R(t) = \frac{\sigma(t)}{\varepsilon_0}}$$



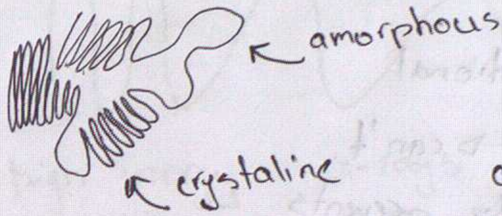
$T_1 < T_2 < T_3 < T_4$

Take E_R at specific time and temp.



- Polymers behave both elastically (instantaneous) and viscously → viscoelasticity

- upon heating a semicrystaline polymer, the glass transition temperature (Tg) corresponds to // is when chains can overcome weak intermolecular forces in amorphous region.

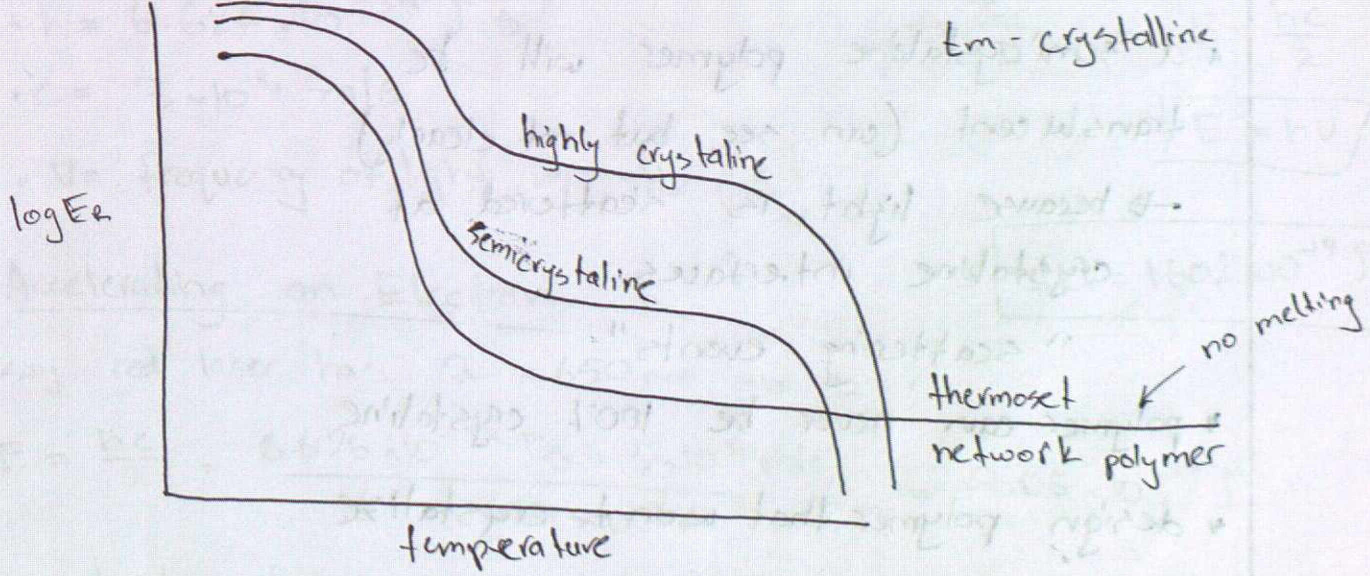


- at melting temperature (tm), molecules can overcome intermolecular forces in crystaline region.

Thermosets and Thermoplastics

tg - amorphous

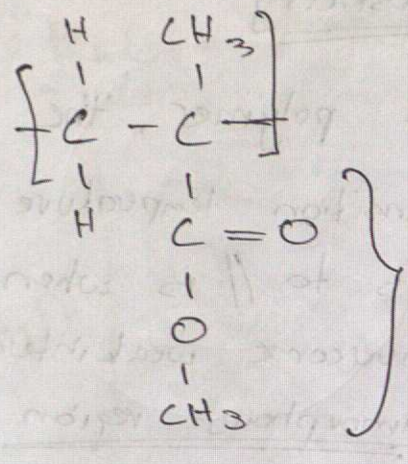
tm - crystalline



Network	highly crystaline
(cannot melt)	will melt
thermoset	thermoplastik

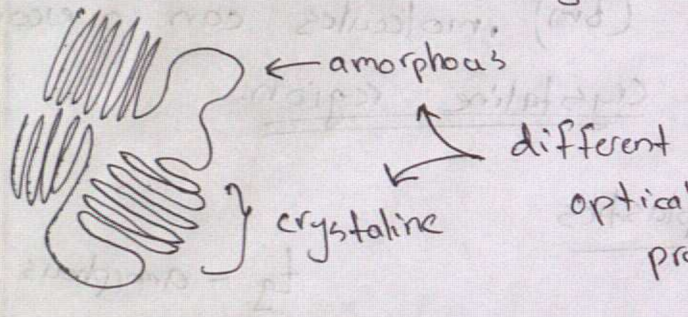
Lec 20

Transparency of Plexiglas®



PMMA is amorphous

bulky functional group → can't stack closely, prevents crystalization



- a semicrystaline polymer will be translucent (can see, but not clearly)
  → because light is scattered at crystaline interfaces
  "scattering events"
- polymer can never be 100% crystaline
- design polymer that won't crystalize

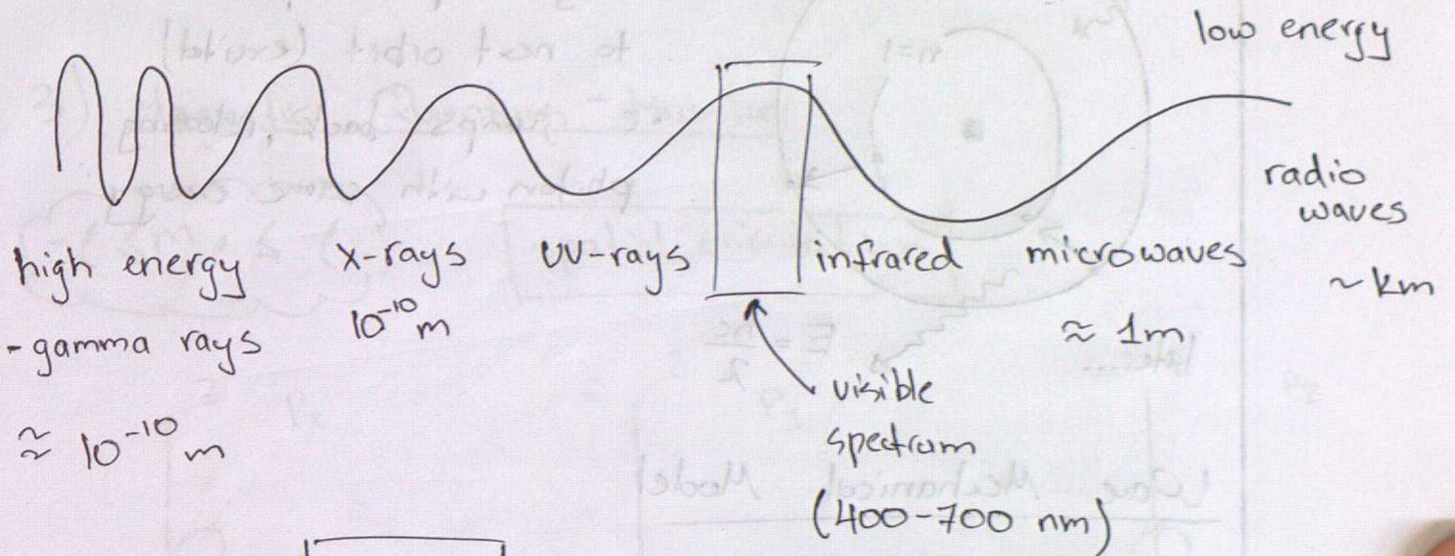
ex sapphire (Al_2O_3) - clear & transparent (crystaline)
window glass - clear & and transparent (amorphous)
metal
- polycrystaline → opaque
- glassy metals → opaque

Ch.9 | Lec 20

Electromagnetic Spectrum

- photon energy $\boxed{E = \frac{hc}{\lambda}}$

h: Planck's constant
c: speed of light
λ: wavelength



Electron $\boxed{E = h\nu}$ 2-3eV

- $h = 6.626 \times 10^{-34}$ J·s
- $c = 3 \times 10^{8}$ m/s
- ν = frequency of light in Hz $(\frac{1}{s})$

$\nu = \frac{c}{\lambda}$, so $E = \frac{hc}{\lambda}$

$\boxed{E = h\nu}$

$\boxed{1eV = 1.602 \times 10^{-19} J}$

Accelerating an Electron

say red laser has λ = 650 nm, so E=?

$$E = \frac{hc}{\lambda} = \frac{6.626 \times 10^{-34} J \cdot s \times 3 \times 10^{8} m/s}{650 \times 10^{-9} m} = 3.06 \times 10^{-19} J$$

- accelerate electron through potential diff. of $1V = \frac{1J}{C}$
- e^- accelerated through 1 V = 1 electon volt of energy, or 1eV

$$1eV = E_{(1e^- \text{ through } 1V)} = \underbrace{1.602 \times 10^{-19} C}_{\text{charge of } e^-} \times 1\frac{J}{C} = 1.602 \times 10^{-19} J$$

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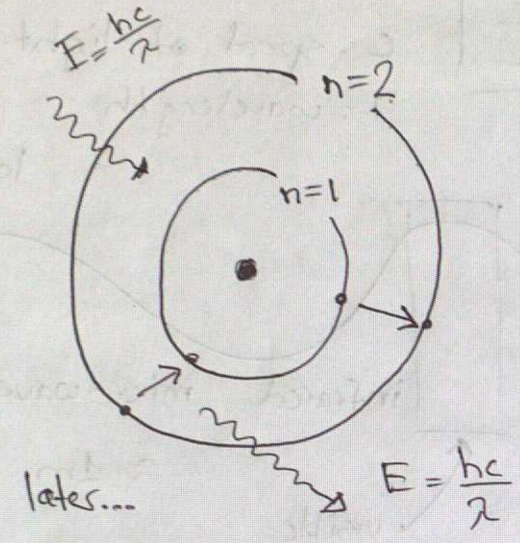
Bohr Model



- Energy is quantized
- e^- gains photon, promoted to next orbit (excited)
- e^- jumps back, releasing photon with same energy

Wave Mechanical Model

4 Quantum Numbers (Q.N.) to describe electron energy

1) Principal Quantum Number

$n = 1, 2, 3, \ldots$ (K L M N ...)

→ describes $\boxed{\text{size}}$ of electron probability distribution

2) Angular Momentum Quantum Number

or

Azimuthal Quantum Number

$l = 0, 1, 2, \ldots (n-1)$ (s p d f)

$\boxed{\text{shape}}$

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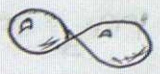
ex shapes

$l = 0 = s$ → sphere 

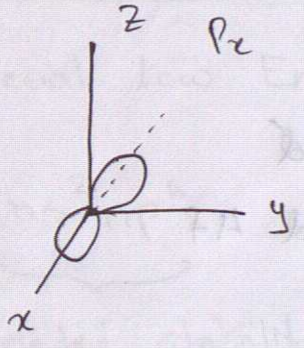
$l = 1 = p$ → dumbell 

ⓘ "s" – sharp
p – principal
d – diffuse
f – fundamental

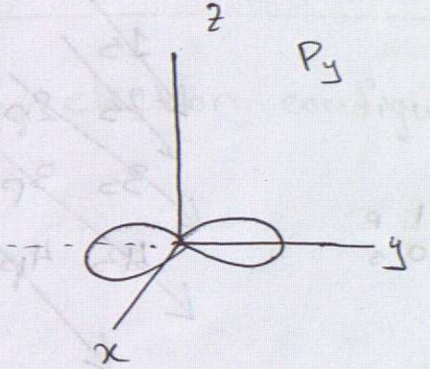
3) Magnetic Quantum Number

$-l \leq m_l \leq l$

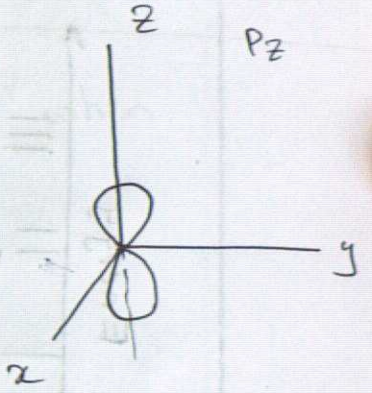
$\boxed{\text{spatial orientation}}$



$m_l = -1$



$m_l = 0$



$m_l = 1$

ex $l = 1$ or p

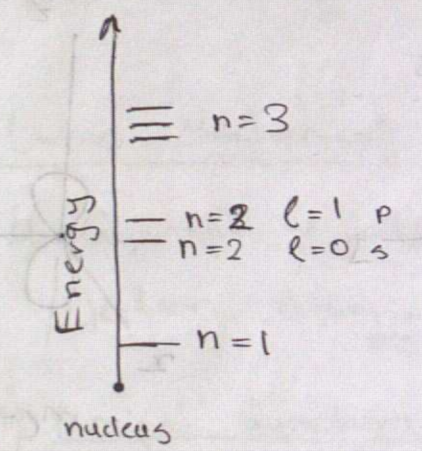
m_l	-1	0	1
p	↑↓	↑↓	↑↓

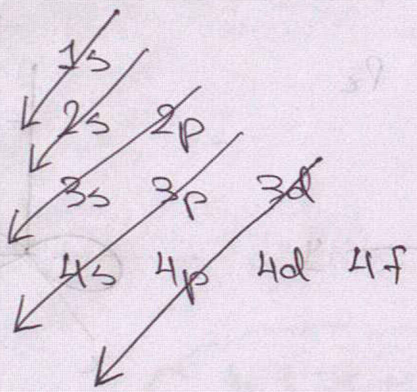
4) Spin Quantum Number

$\boxed{\text{spin}}$ $m_s = +\frac{1}{2}$ or $-\frac{1}{2}$

Relative Energy Levels

(isolated atom)





ex Carbon proton # (Z) = 6

need 6 electrons

$1s^2 2s^2 2p^2$

	how many e^- hold?
s	2
p	6
d	10
f	14

ex Iron Z = 26

$1s^2 2s^2 2p^6 3s^2 3p^6 \cancel{4s}^2 \cancel{3d}^6$

$3d^6 4s^2$

---

ex Fe^{2+}

rule of thumb for ions: ionize highest principal Q.N. first

$Fe^{2+}: \underbrace{\underbrace{\underbrace{1s^2}_{[He]} 2s^2 2p^6}_{[Ne]} 3s^2 3p^6}_{[Ar]} 3d^6 \longrightarrow [Ar]\,3d^6$

Special Low Energy electron configuration when

$\underbrace{ns^2 np^6}_{\text{octet stability}}$

Exceptions

chromium: $1s^2 2s^2 3p^6 3s^2 3p^6 3d^5 4s^1$

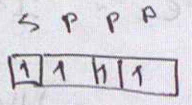
copper: $1s^2 2s^2 3p^6 3s^2 3p^6 3d^{10} 4s^1$

Primary ("strong") Bonds

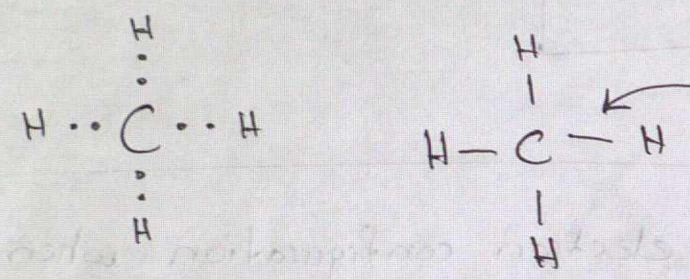
1) **Covalent** (sharing of electrons)

ex CH_4 C z=6 : $1s^2 2s^2 2p^2$ →

H z=1 : $1s^1$



sp^3 hybridization



covalent bond

directional

one H only attracted to specific C

2) **Ionic** (transfer of electrons)

ex NaCl Na z=11 : $\underbrace{1s^2 2s^2 2p^6}_{\text{almost stable octect}} 3s^1$ } get rid

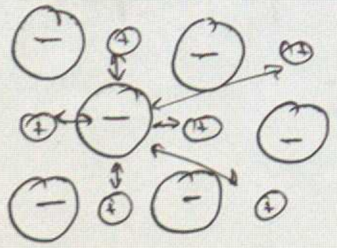
Cl z=17 : $1s^2 2s^2 2p^6 \underbrace{3s^2 3p^5}_{\text{almost stable octet, need } 1e^-}$

2 logical steps

1) electron transfer to achieve low energy e^- config.

↳ Na^+ and Cl^-

2) charge attraction (coulombic attraction)



non-directional

attracts all opp. chage atoms

---

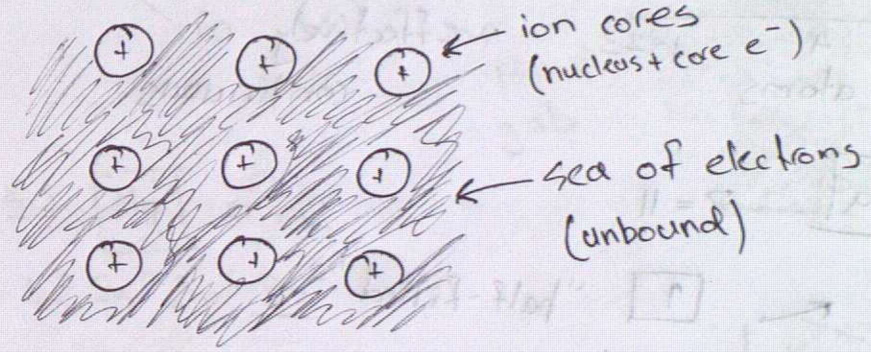
3) Metallic

↳ outermost e^- (valence electrons) are contributed to "sea of electrons"

↳ delocalized, not bound to a specific nucleus

↳ core electrons remain bound to nucleus

↳ ion core



- explains electrical conductivity
- explains ductility

Why salt a Crystal?

$Na(s) + \frac{1}{2}Cl_2(g) \longrightarrow NaCl(s)$

Na

1. $Na(s) \longrightarrow Na(g)$ $\Delta H = 109 \frac{kJ}{mol}$ (sublimation)
2. $Na(g) \longrightarrow Na^+(g) + e^-$ $IE_{Na} = 497$ kJ/mol (ionization)

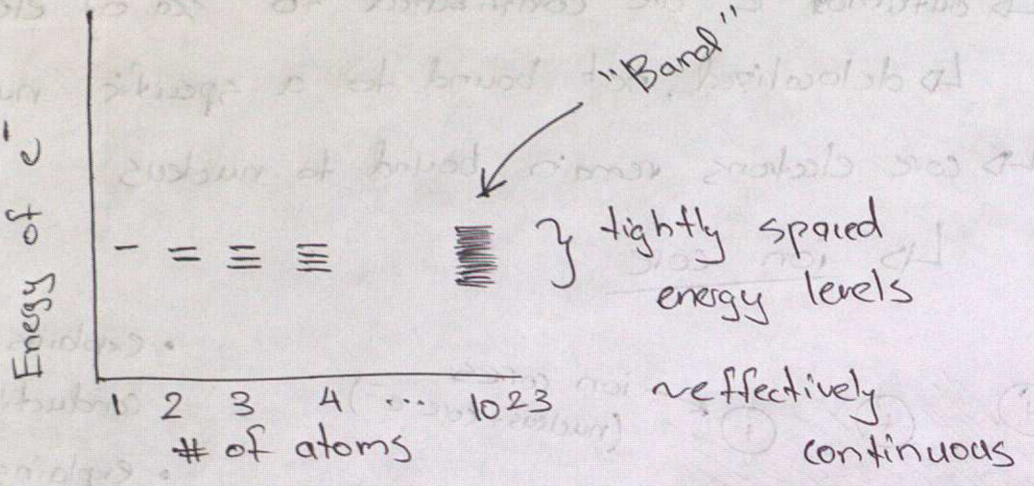
Cl

1. $\frac{1}{2}Cl_2(g) \longrightarrow Cl(g)$ BDE = 121 kJ/mol (bond dissociation)
2. $Cl(g) \xrightarrow[+e^-]{} Cl^-(g)$ $EA_{Cl} = -364$ kJ/mol (e^- affinity)

crystalization

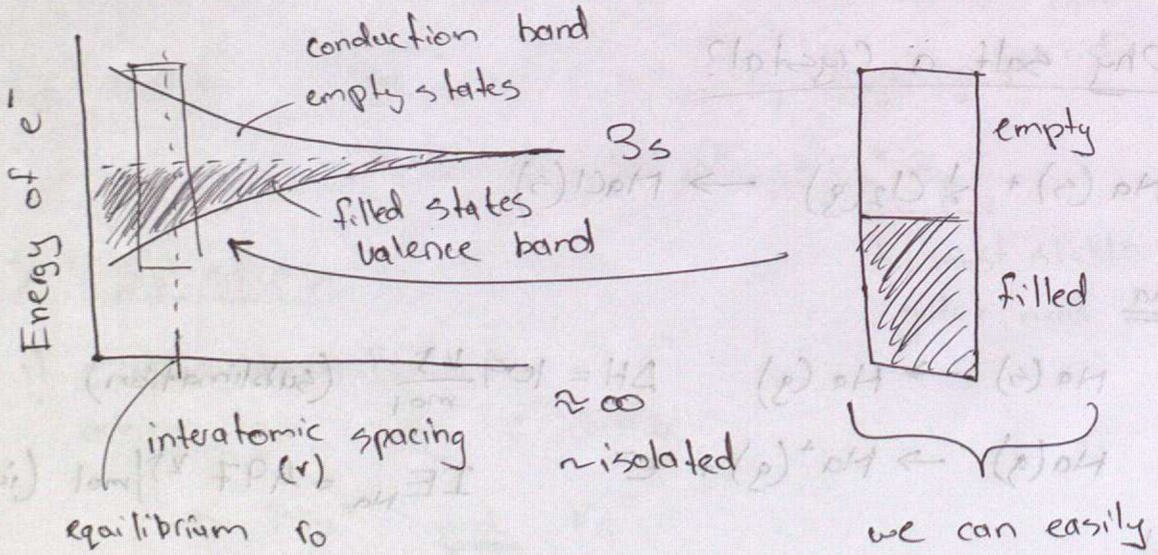
$Na^+(g) + Cl^-(g) \longrightarrow NaCl(s)$ $E_{cryst.} = -777$ kT/mol

Band Theory of Solids

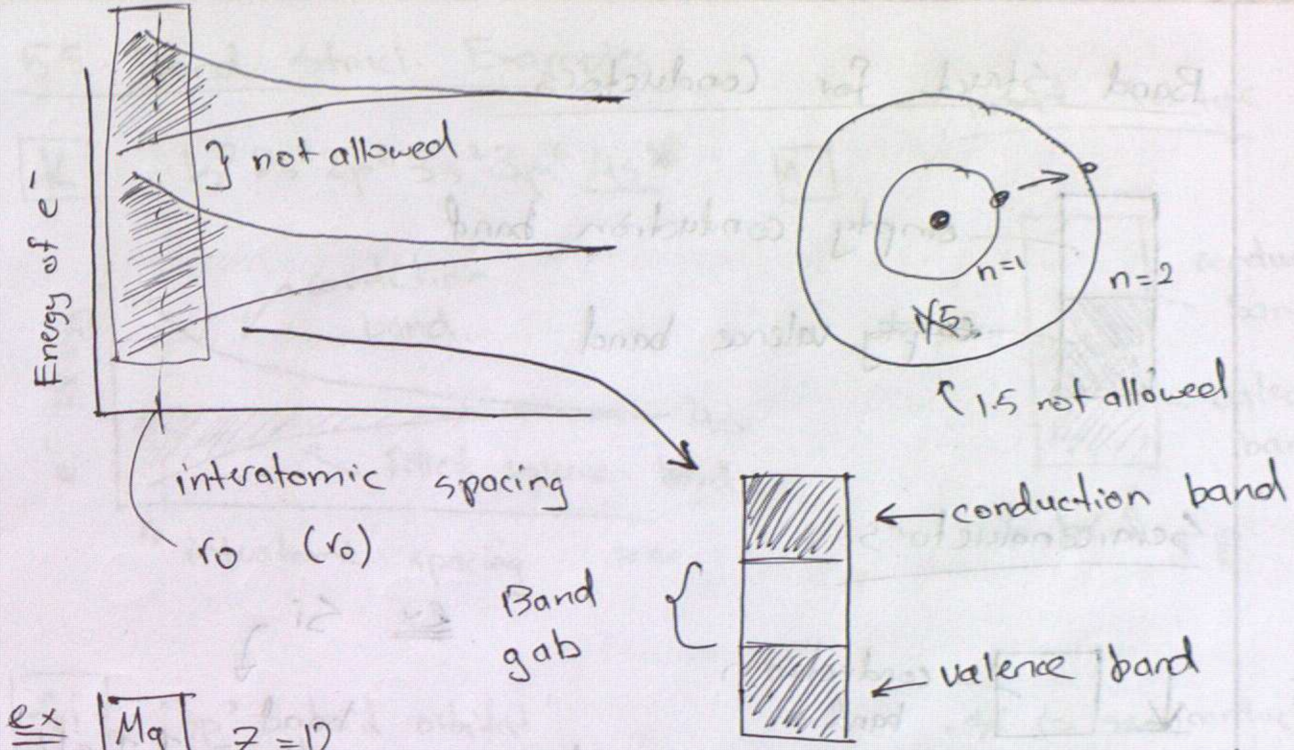


ex metallic $\boxed{Ha}$ $Z = 11$

$1s^2 2s^2 2p^6 \underline{3s^1}$ ← $\boxed{\uparrow}$ "half-filled"



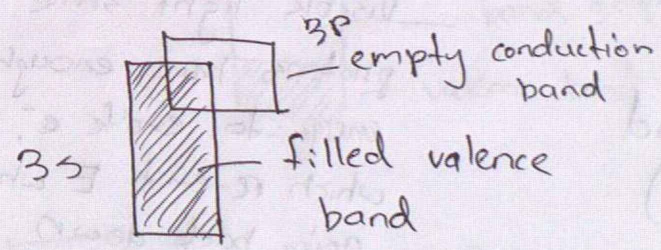
we can easily promote an electron to a higher energy level (conduction band)

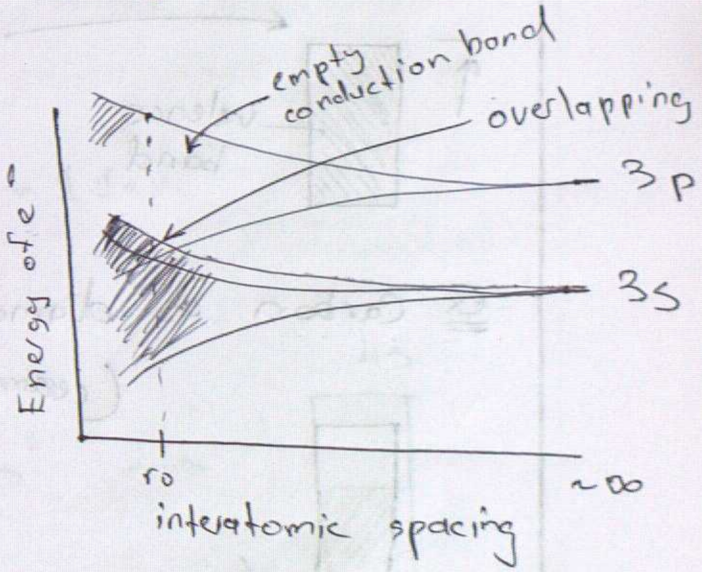


ex $\boxed{Mg}$ $Z = 12$

$1s^2 2s^2 2p^6 \underline{3s^2}$

Band structure

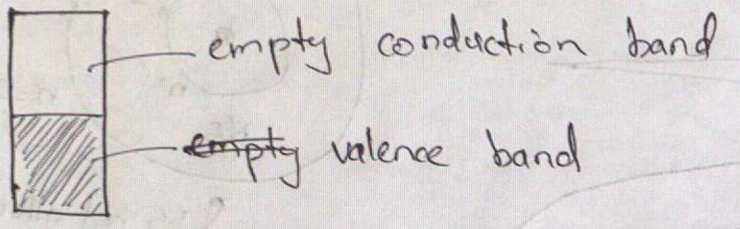




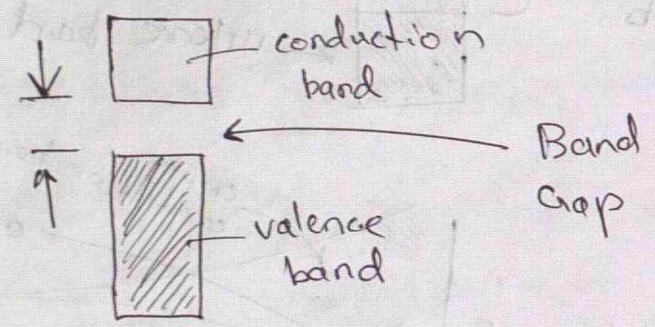
$\boxed{Mg}$ is conductive!

- "filled" 3s energy level in fact includes some empty 3p energy levels, since they're overlapped.

Band Struct. for Conductors



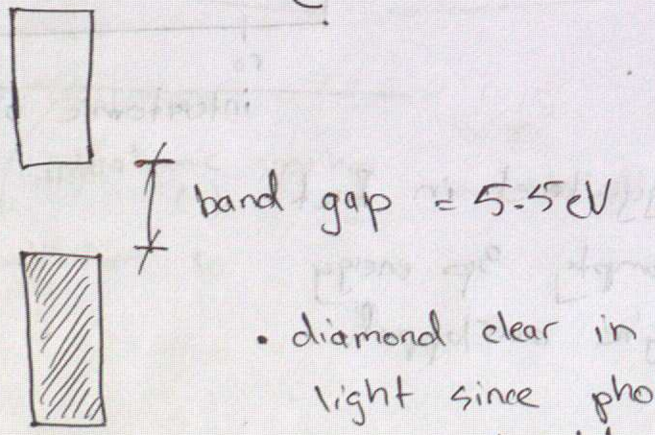
Semiconductors



ex Si → band gab = 1.1 eV

- Si is shiny in visible light since photons have enough energy to excite e^-, which re-emit E when going back down

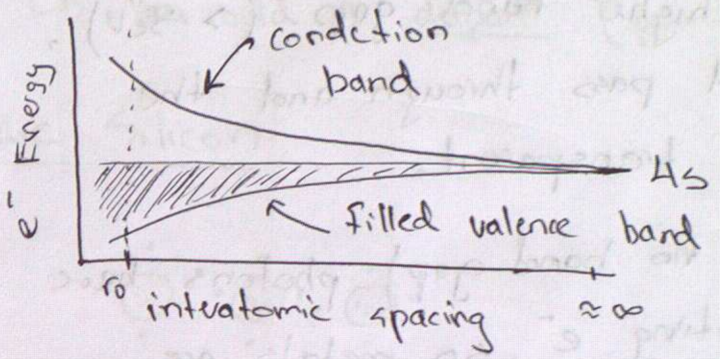
ex Carbon as diamond (ceramic)

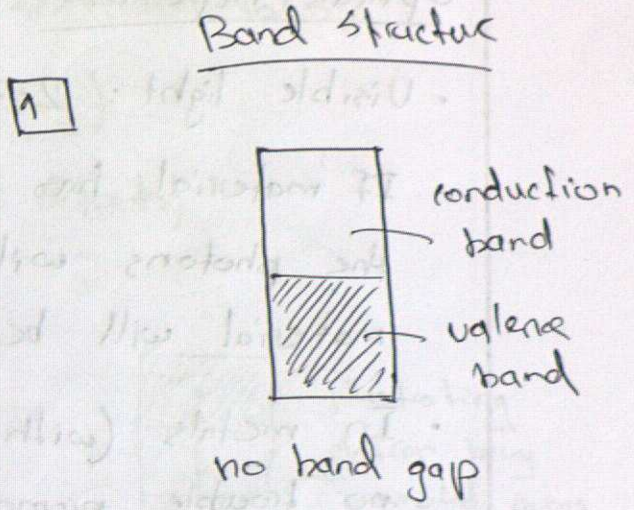


- diamond clear in visible light since photons pass straight through without promoting e^-

55 - Band Struct. Examples

K $1s^2 2s^2 2p^6 3s^2 3p^6 \underline{4s^1}$

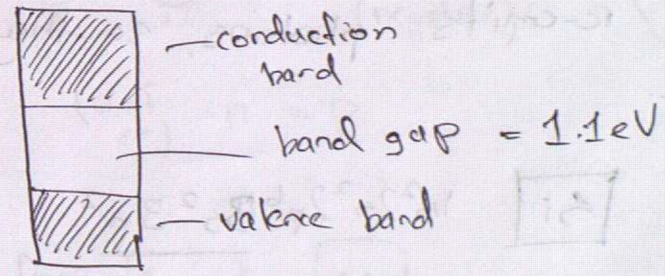




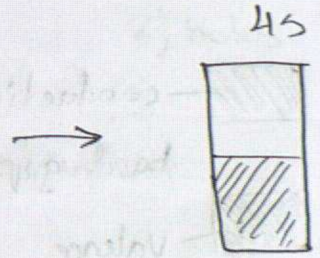
no band gap

Si "sp^3 hybrid orbital"

- Si is semiconductor



Cu $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^1$ →



No band gap → conductor 

band gap > 4eV → insulator 

band gap < 4eV → semiconductor 

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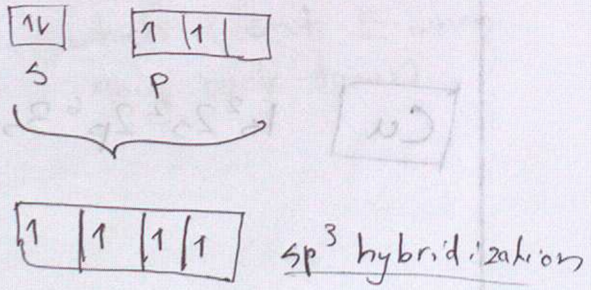
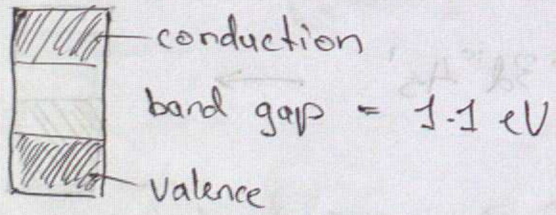
Optical Properties

- Visible light : 2-3 eV
- If material has higher band gap (> 3eV), the photons will pass through and the material will be transparent.
- In metals (with no band gap), photons have no trouble promoting e^-, so metals are opaque (not transparent)
- Electons in metals dropping to original energy levels re-emits photons, so they are shiny.

Semiconductors

$\boxed{Si}$ $1s^2 2s^2 2p^6 \underline{3s^2 3p^2}$





Polymess : covalent bond, no e^- free to conduct

Cesamics : ion attraction, so no free e^-
(ionic)

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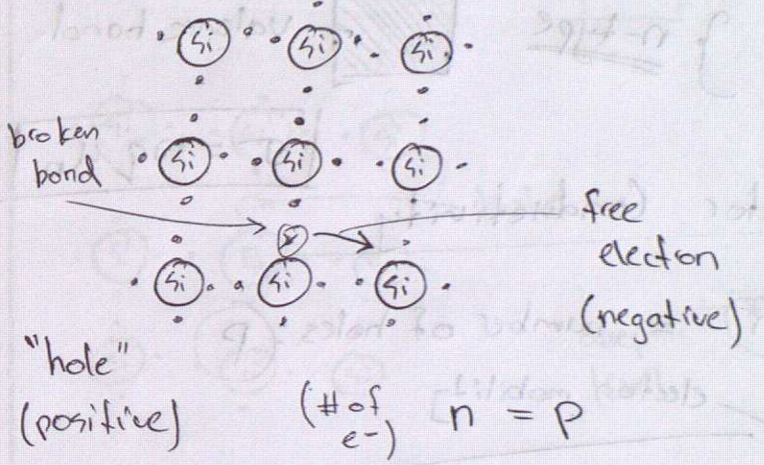
How to control conductivity in semiconductors?

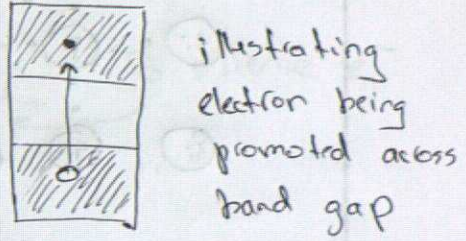
↳ by adding impurities. (doping)

↳ You add a <u>dopant</u> (point defects)

Pure Silicon



(# of e^-) $n = p$

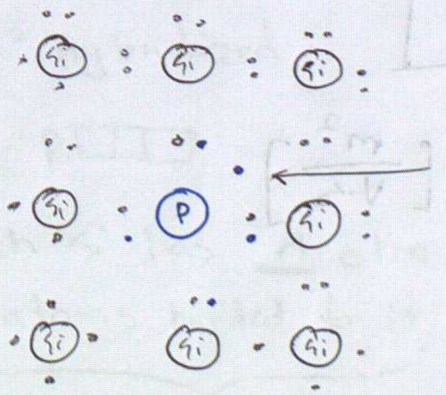


Intrinsic Semiconduction

↳ 2 charge carriers
1) electons n
2) holes p

Adding Dopants to $\boxed{Si}$

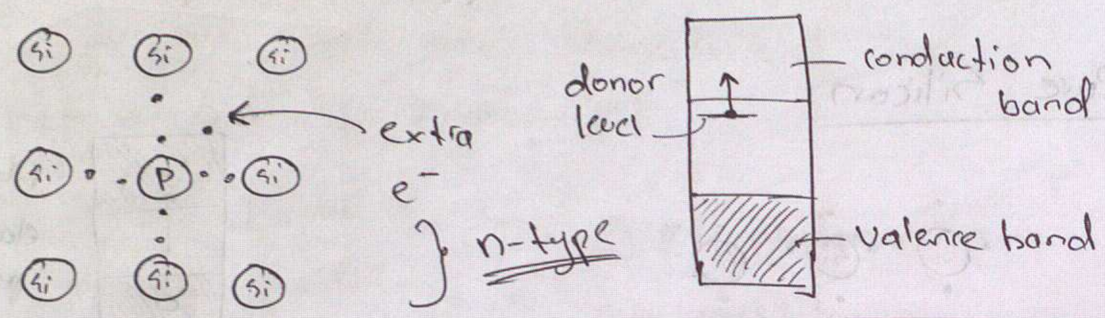
ex $\boxed{P}$ $1s^2 2s^2 2p^6 \underbrace{3s^2 3p^3}$ ← pentavalent



charge carrier
↳ negative

n-type
extrinsic

Adding impurities (point defects) to $\boxed{Si}$ (doping) to form Extrinsic Semiconductor



$$\boxed{\sigma = nq\mu_n}$$

Intrinsic Semiconductor Conductivity

number of e⁻'s : ⓝ = number of holes : ⓟ

electon mobility

$$\boxed{\sigma = n \cdot q\mu_n + p \cdot q\mu_p}$$

conductivity

\# of electons

fundmental charge

hole mobility

$$\boxed{\sigma = nq(\mu_n + \mu_p)}$$

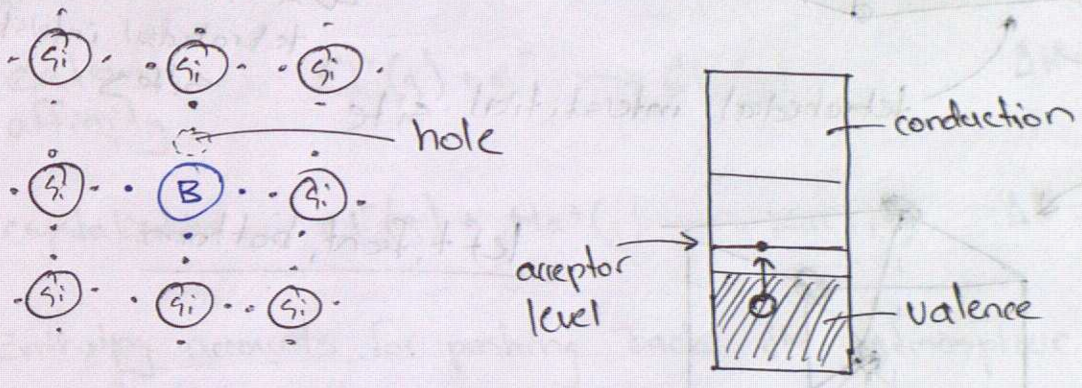
$[\Omega^{-1}m^{-1}]$ $[\#]$ $[C]$ $\left[\frac{m^2}{V \cdot s}\right]$

N-Type Extrinsic Semiconductor Conductivity

$$\boxed{\sigma = nq\mu_n}$$

P-Type Extrinsic Semiconductor

- Dope with Boron $\boxed{B}$ $1s^2 2s^2 2p^1$ ← 3 valence e⁻



$$\boxed{\sigma = pq\mu_p}$$

Diamond Cubic Crystal Structure

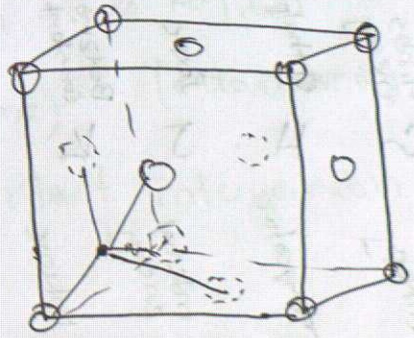
ex $\boxed{Si}$, $\boxed{C}$ (as diamond)

- sp^3 hybridized

s☐ p☐☐☐

- each Si has 4 other Si atoms bonded to it

$\underbrace{\hphantom{each Si atoms bonded to it}}_{\text{tetrahedral site}}$



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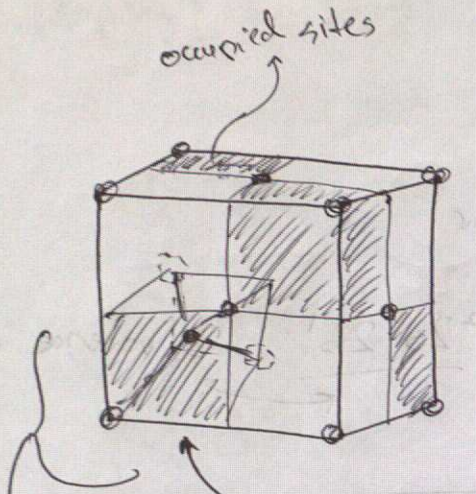
Diamond Cubic

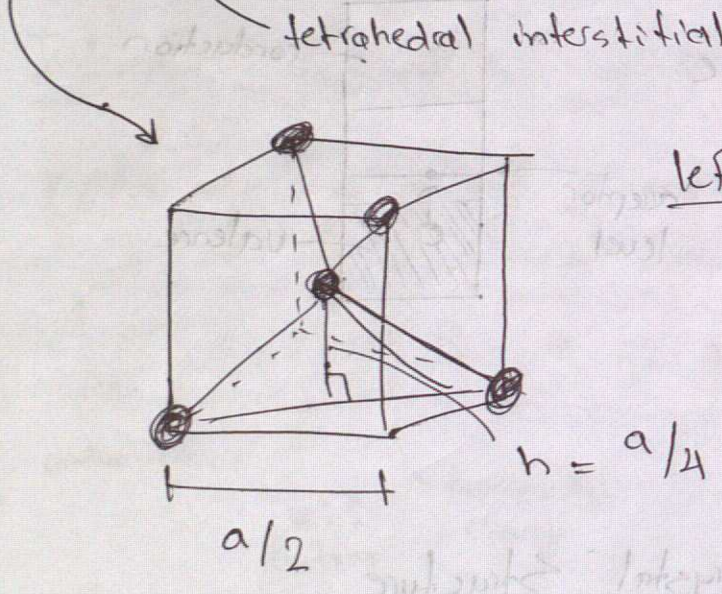


- Sliced into 8 - subcubes
- only 4 of the subcubes are populated

$n_{\text{Diamond cubic}} = 8$

↳ 4 from FCC

↳ 4 from inside tetrahedral interstitial sites



left, front, bottom

Thermodynamic Alphabet

G	Gibbs energy
H	enthalpy
J	Joule
K	Boltzmann constant
L	litre
M	mass
N	# of moles
P	pressure
q	heat
R	gas constant
S	entropy
T	temperature
U	internal energy
V	Volume
W	work

Ch.10 | Lec 25

Salt as Crystal

let's start with : $Na(s) + \frac{1}{2} Cl_2(g) \longrightarrow NaCl(s)$

sublimation	$Na(s) \rightarrow Na(g)$	$\Delta H = 109 \frac{kJ}{mol}$
ionization	$Na(g) \rightarrow Na^+ + e^-$	$\Delta H = 497 \frac{kJ}{mol}$
bond dissociation	$1/2\, Cl_2(g) \rightarrow Cl^*(g)$	$\Delta H = 121$ kJ/mol
electron affinity	$Cl^*(g) + e^- \rightarrow Cl^-(g)$	$\Delta H = -364$ kJ/mol
crystalization	$Cl^-(g) + Na^+(g) \longrightarrow NaCl(s)$	$\Delta H = -777 \frac{kJ}{mol}$

- Enthalpy accounts for pushing back the atmosphere

Total = −414 kJ/mol → heat out , exothermic

doesn't necessarily mean the rxn will happen

- Thermodynamics : achieving low energy
- Kinetics : how fast something will happen

ex $H_2O(s) \longrightarrow H_2O_{(l)}$ $\Delta H = +6$ ~~4~~ kJ/mol (endothermic)

Spontaneous (in thermodynamic sense)

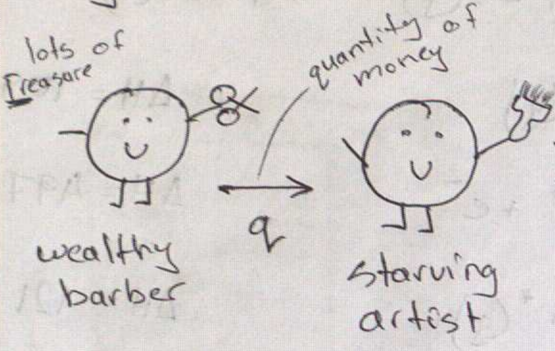
↳ rxn proceeds without constant interversion.

↳ (not necessarily fast)

↳ does not mean "for no apparent reason"

Spontaneous Reaction

say we observe a town



First law of thermody.

we observe:

1) money is not printed

2) Artist never gives money to barber spontaneously

$\underbrace{\quad}$ Second law of thermodynamics

We can define Something for the town

$S = \frac{q}{T}$

↗ entropy

Only transactions where

$$\boxed{\Delta S_{Town} = \Delta S_B + \Delta S_A > 0}$$

entropy of universe

Does this work?

1) Barber gives money to artist

$\Delta S_{Town} = \Delta S_B + \Delta S_A$

$= \frac{-q}{T} + \frac{q}{T} > 0$ YES!

satisfies above laws, so...

$=$ small negative $+$ positive larger

2) Artist transfers money to barber (cool coffee → becomes hot coffee)

$\Delta S_{Town} = \frac{q}{T} + \frac{-q}{T}$

$=$ small positive $+$ large negative < 0 NO

does't comply with law, so...

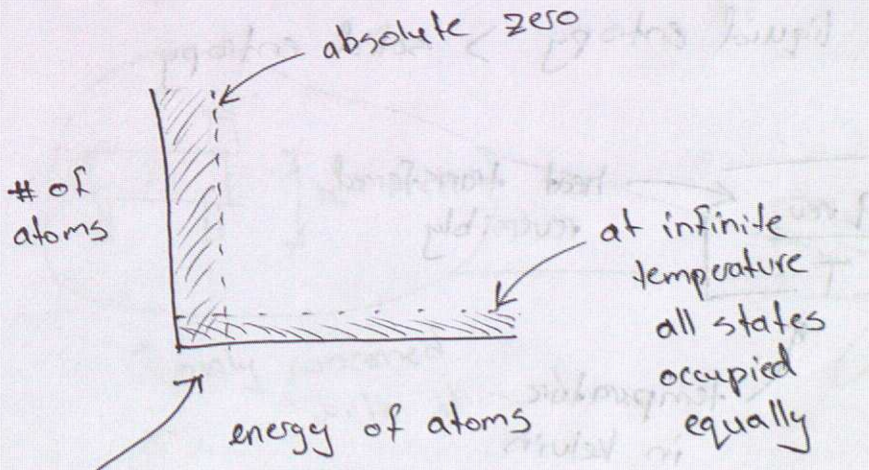
3) Artist pays Barber for haircut

↳ Yes, if driven by a good haircut } AC powered by increase in entropy in power plant

Second Law of Thermodynamics

$$\boxed{\Delta S_{universe} \text{ must increase for a spontaneous rxn.}}$$

* entropy sometimes described as meaure of disorder



at infinite temperature all states occupied equally (maximum entropy) ← more uncertanty about what energy a given atom has

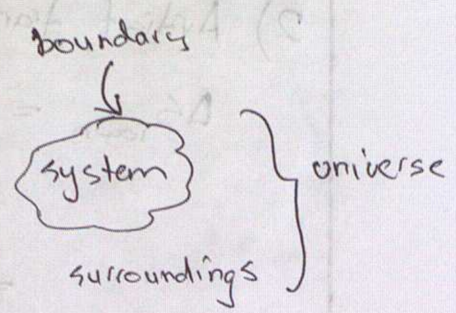
lowest energy state (zero entropy)

↑ no uncertainty about what energy an atom has → since you know they're all in lowest energy state.

- entropy is an indication of how accurately you can predict the energy that any given atom would have

2nd Law of Thermodynamics

$\Delta S_{universe} = \Delta S_{sys} + \Delta S_{surr} > 0$



- Entropy sometimes described as "disorder"
- Entropy describes the uncertainty in knowing precisely the energy that an atom/molecule will have.

Entropy as Disorder

A system at high entropy → highly disordered (You can't predict where anything is)

gas entropy > liquid entropy > solid entropy

$$\boxed{\Delta S = \frac{q_{rev}}{T}}$$

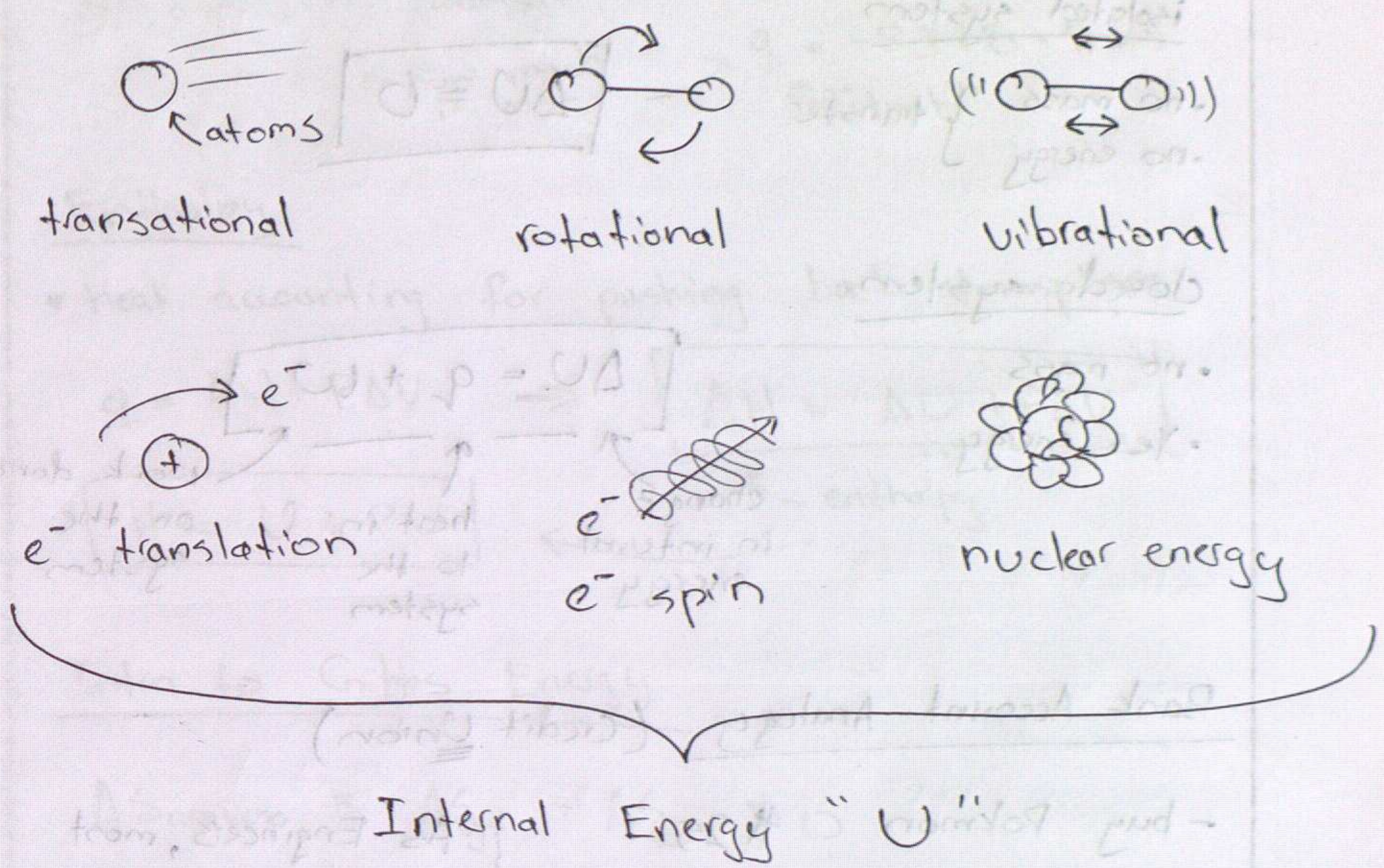
← heat transferred reversibly

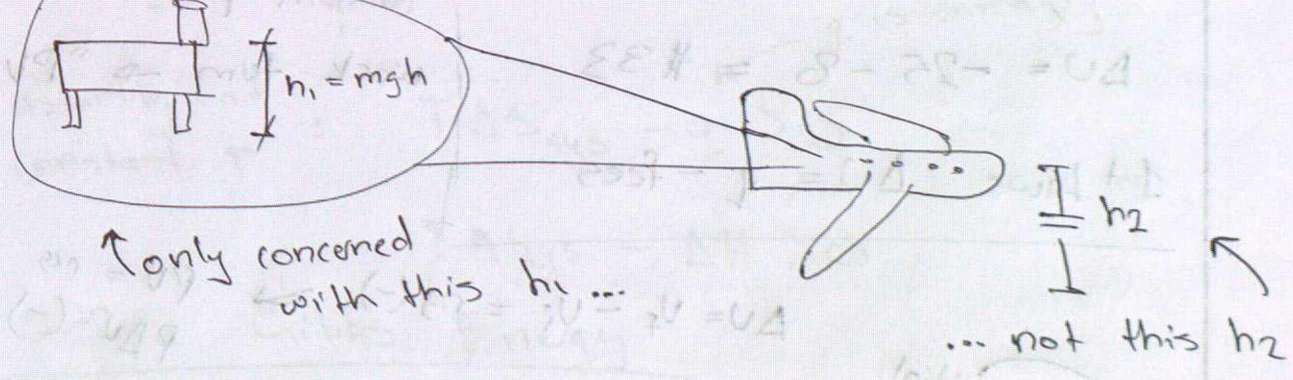
entropy ↗

↖ temperature in kelvin

* Total entropy change ($\Delta S_{universe}$) for universe must be positive (>0) for a process to be spontaneous.

Microscopic Energy





$\boxed{\text{Thermodynamics is concerned with } \Delta U \leftarrow \text{internal energy change}}$

1st Law of Thermodynamics

isolated system

- no mass } transfer
- no energy

$$\boxed{\Delta U = 0}$$

closed system

- no mass
- Yes energy

$$\boxed{\Delta U = q + \omega}$$

change in internal energy

heat in to the system

work done on the system

Bank Account Analogy (Credit Union)

- buy Pokmon $25
- pay shipping fees $8

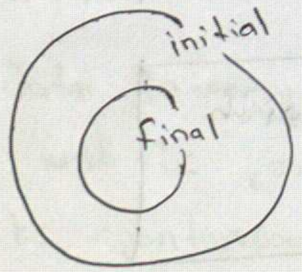
$\Delta U = -25 - 8 = \$33$

1st Law: $\Delta U = q - \text{fees}$

As Engineers, most processes are at constant pressure... work term → "PV"

$\Delta U = U_f - U_i = neg(-) \Rightarrow PV = neg$

$P\Delta U = (-)$



1st Law becomes

$$\boxed{\Delta U = q - P\Delta U}$$

Case I forgot q

$\Delta U = -33\$$ ← charge on account

how much it cost

pokemoncost

$q = \Delta U + \text{fees}$

$q = -33 + 8 = \$25$

"heat"

Enthalpy

- heat accounting for pushing back atmosphere

$q = \Delta U + P\Delta U \Rightarrow \boxed{\Delta H = \Delta U + P\Delta U}$

enthalpy

$$\boxed{H = U + PV}$$

Intro to Gibbs Energy

$\Delta S_{universe} = \Delta S_{sys} + \Delta S_{surr} > 0$

$\Delta S_{syst} + \frac{-q}{T}$

q is enthalpy

assuming at constant T: $T\Delta S_{sys} - q > 0$

$T\Delta S_{sys} - \Delta H > 0$

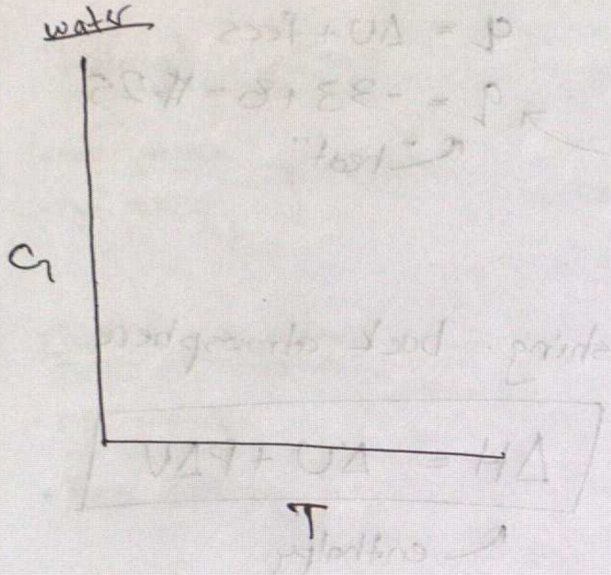
Define Gibbs Energy

$$\boxed{\Delta G = \Delta H_{sys} - T\Delta S_{sys}}$$

only in terms of system

Ch-11 |Lec 27

Plot H − TS ⟹ $G = H - TS$



path function

$P, q, S, T, U, V, \omega, H$

state functions

Standard State

→ the most stable form of a pure element at 25°C and 10^5 Pa (298.15 K and 1 atm)

ΔH vs ΔU ?

ex $2C_8H_{18}(l) + 25O_2(g) \rightarrow 18H_2O(g) + 16CO_2(g)$

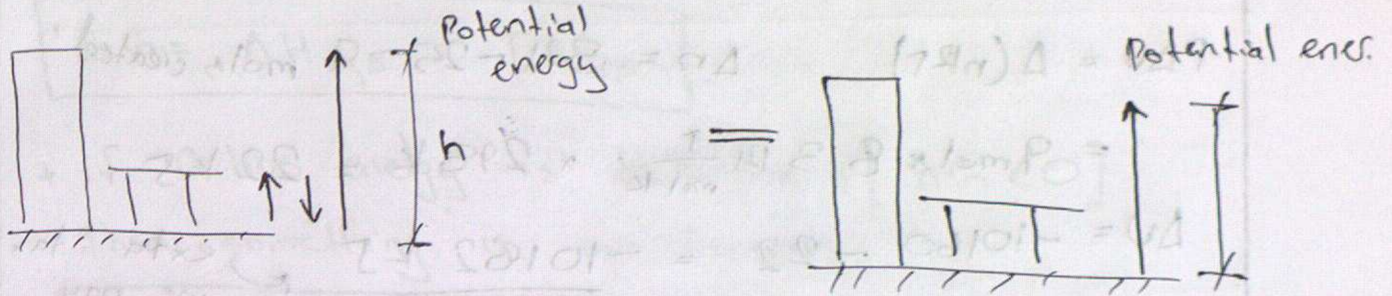
- need a reference point to measure changes against.
- ΔH only depends on current condition
  ↳ doesn't depend on how it got there

$\boxed{\text{State function}}$ G, S, H

$\underbrace{\text{heat, work are not state functions}}_{\text{Path function}}$

Ch-11

Standard State



- all that matters is final height, since...
- potential energy is a state function
  ↳ doesn't matter how we got to state, all that matters is what that state is

Path functions: work

State funtions: temperature, PE, enthalpy, internal energy

Difference Bt. U and H

$2C_8H_{18}(l) + 25O_2(g) \rightarrow 18H_2O(g) + 16CO_2(g)$

$$\Delta H^\circ_r = \Delta H^\circ_{form}(CO_2(g)) \cdot 16 + \Delta H^\circ_{form}(H_2O(g)) \cdot 18 - \Delta H^\circ_{form}(C_8H_{18}(l)) \cdot 2 - H^\circ_f(\cancel{O_2(g)}) \cdot 2 \rightarrow 0$$

$\Delta_f H^\circ$ v.s ΔH_f° } enthalpy required to form substance at standard state

↑ IUPAC recommended

ex: $\Delta_f H^\circ \cdot O_2(g) = 0$ KJ/mol

$\Delta_r H^\circ = \Delta_{comb} H^\circ = -10160$ KJ

$\Delta H = \Delta U + P\Delta V \longrightarrow \Delta U = \Delta H - P\Delta V$

$P\Delta V = \Delta(nRT)$ $\Delta n = 34 - 25 = 9$ mols created

$= 9\,mol \times 8.314 \frac{J}{mol\cdot K} \times 298\,K = 22\,kJ$

$\Delta U = -10160 - 22 = \underline{-10182\,kJ}$ ← extra "tax" we pay

- Enthalpy and Internal Energy are basically same for solids, since there is minimal Volume changes
- with gases, be cautious!

Gibbs Energy

$\Delta S_{sys} + \Delta S_{surr} > 0$

$\Delta S_{sys} - \frac{q_{rev}}{T} > 0$ at constant T

$T\Delta S_{sys} - \frac{q}{\cancel{T}} \cdot \cancel{T} > 0$

$T\Delta S_{sys} - q > 0$ at constant P

$-1\,\underbrace{(T\Delta S_{sys} - \Delta H_{sys} > 0)}_{\Delta G}$ } restatement of the 2nd law for constant T, P

"Gibbs energy"

Gibbs Energy

$\boxed{\Delta G = \Delta H_{sys} - T\Delta S_{sys}}$

- if Gibbs energy is decreasing $[\Delta G < 0]$ then something is spontaneous.

$\boxed{\Delta G = \Delta H_{sys} - T\Delta S_{sys} < 0, \text{ then spontaneous}}$

- Gibbs energy decrease means entropy increased

$\boxed{\Delta G = -T\Delta S_{universe}}$

Gibbs Rxns

$\Delta G < 0$ means $\Delta S_{universe} > 0$ "spontaneous"

	ΔH	ΔS_{sys}	Spontaneous?
1)	negative "exothermic"	positive (+)	always
2)	negative (exothermic)	negative (−)	at low temp
3)	positive "endothermic"	positive (+)	at high temp
4)	positive "endothermic"	negative (−)	never

Examples

1) burning fuel
2) freezing water
3) melting ice

Absolute Entropy

The Entropy of any perfect crystal approaches 0 (zero) as temp. approaches zero kelvin (absolute zero)

Third Law of Thermo

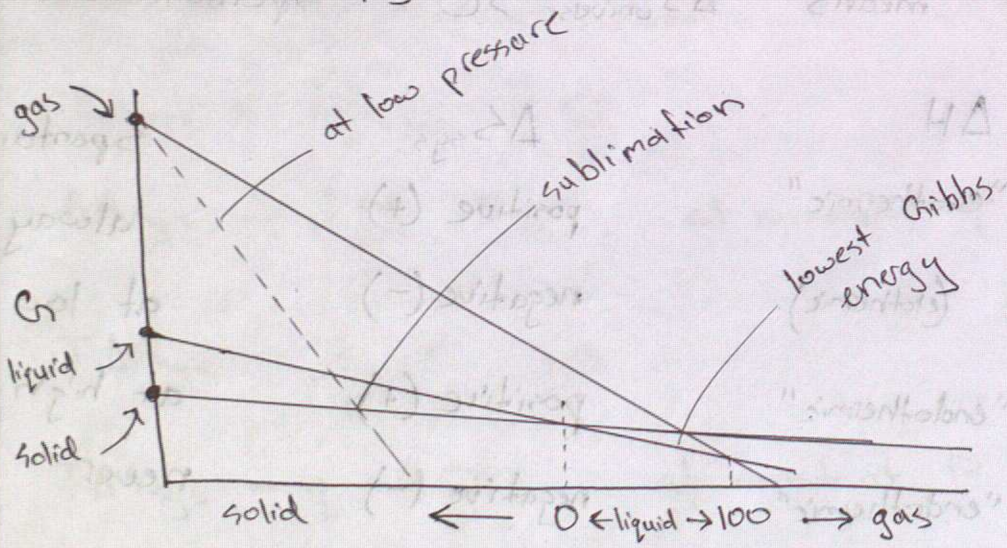
- we can determine absolute value for entropy due to 0 kelvin "reference point" unlike enthalpy, for which we only know change.

Plotting Gibb's Energy for Water

Plot $G = H - TS$

$y = mx + b$

$G = -ST + H$ ← intercept, $-S$ ← slope



S_{solid} v.s S_{liquid}? $\Longrightarrow S_{solid} < S_{liquid} < S_{gas}$

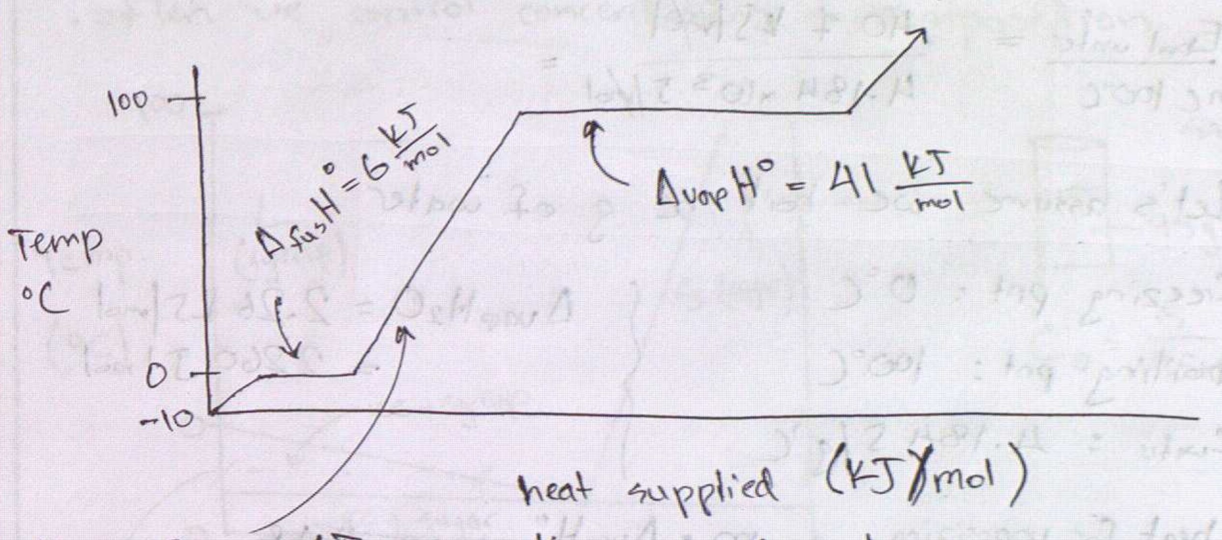
- modern freezers, ice cubes go from solid → gas ... why?
- pressure changes gas "graph slope line" so at low temp, it intersects solid graph slope and exists as gas directly

---

Enthalpy of fusion, vapourization for water

$H_2O_{(s)} \rightarrow H_2O_{(l)}$ "melting" fusion endothermic

$\Delta_r H^\circ = \Delta_{fus} H^\circ = \Delta_f H^\circ(H_2O_{(l)}) - \Delta_f H^\circ(H_2O_{(s)}) = 6\ kJ/mol$



Slope ? $\frac{\Delta T}{q}\ [=]\ \frac{K}{kJ/mol} = \frac{K \cdot mol}{kJ}$

calculate heat transferred : $q = \frac{1}{slope} \times \Delta T$

$\left[\frac{J}{mol}\right] \rightarrow \boxed{q = n\, C_p\, \Delta T}$

# of mols

molar heat capacity $\left[\frac{J}{mol \cdot K}\right]$

temperature change $[K]$

OR

$\boxed{q = mc\Delta T}$

mass

specific heat capacity $\left[\frac{J}{g \cdot K}\right]$

Ch.11

Q.11.15.1

$$\frac{E_{\text{boil water}}}{E_{0°C \to 100°C}} = \frac{mc\Delta T}{mc\Delta T}$$

$$\frac{E_{\text{boil water}}}{mc\,100°C} = \frac{40.7\ kJ/mol}{4.184 \times 10^3\ J/mol} =$$

Let's assume we boil x g of water

freezing pnt : 0°C

boiling pnt : 100°C

C_{water} : 4.184 J/g°C

$\Delta_{vap}H_2O = 2.26\ kJ/mol$
$= 2260\ J/mol$

$$\frac{\text{heat for vaporizing}}{\text{E for freezing} \to \text{boil}} = \frac{m \cdot \Delta_{vap}H^\circ}{m \cdot C \cdot \Delta T} = \cancel{m = 4.18}$$

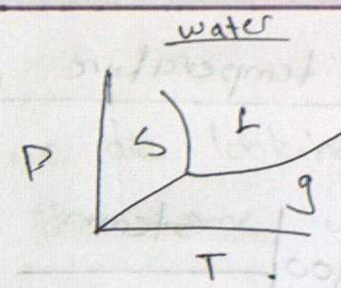
$$= \frac{m \cdot 2260\ J/mol}{m \cdot (4.184\ J)(100°C)} = \frac{2260}{418.4} \approx 5.4$$

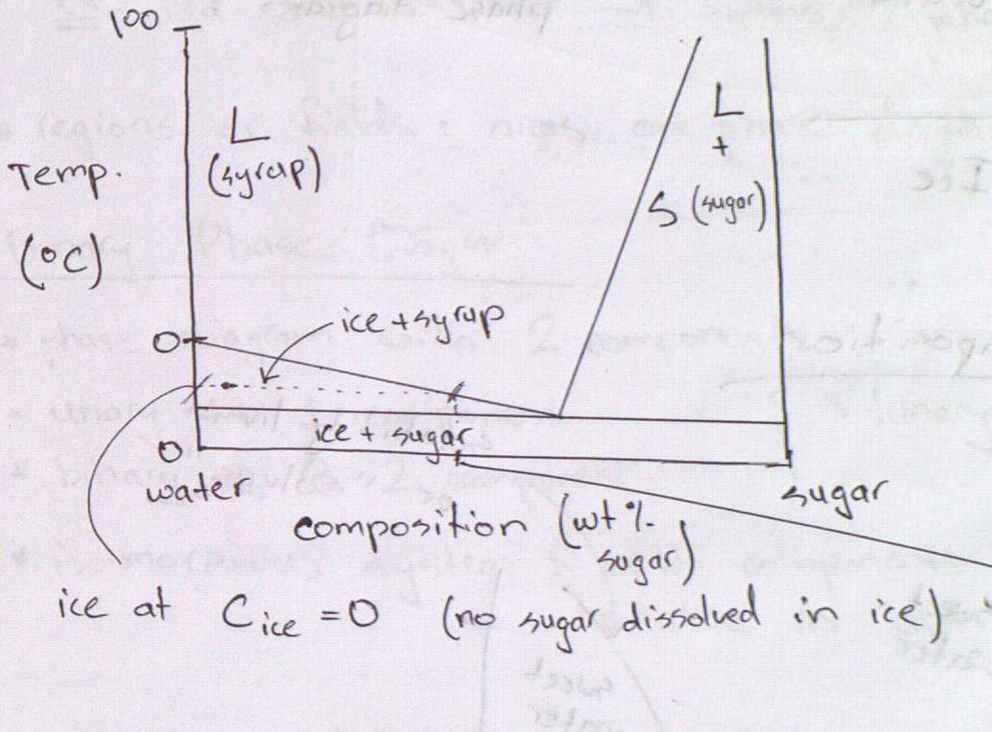
≈ 6

Ch.12 / Lec 30

Phase Diagrams

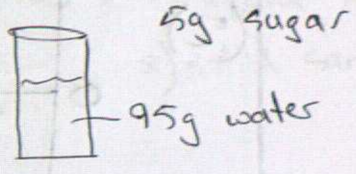
- convey phase stability
- normally P = 1 atm
- often we control concentation = composition



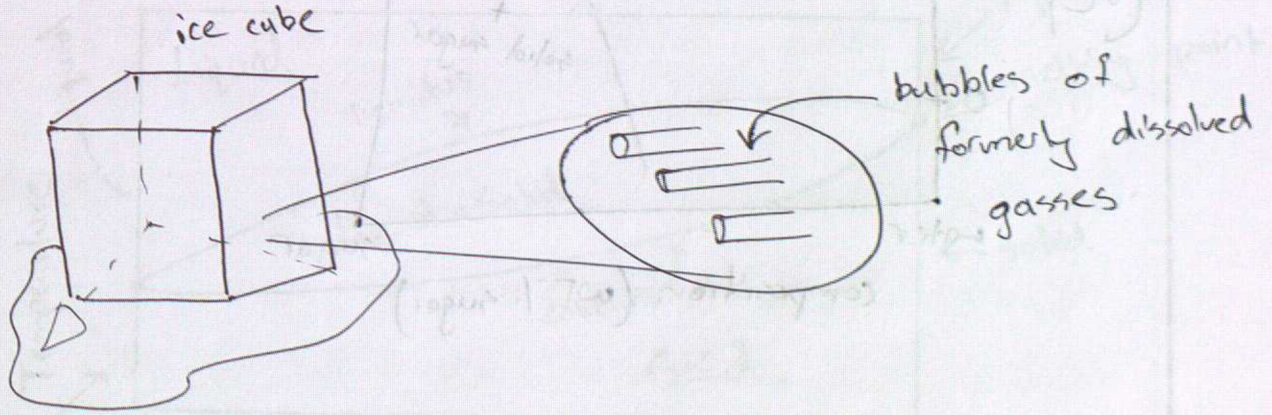


ice at $C_{ice} = 0$ (no sugar dissolved in ice)

syrup at $C_{syrup} = 45$ wt%.

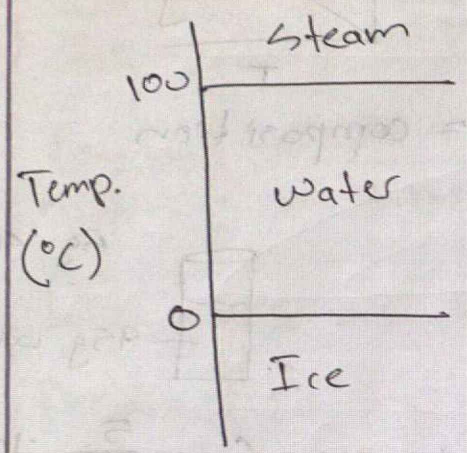


$$C_0 = \frac{5}{95+5} \cdot 100\% = 5\ \text{wt\%}$$



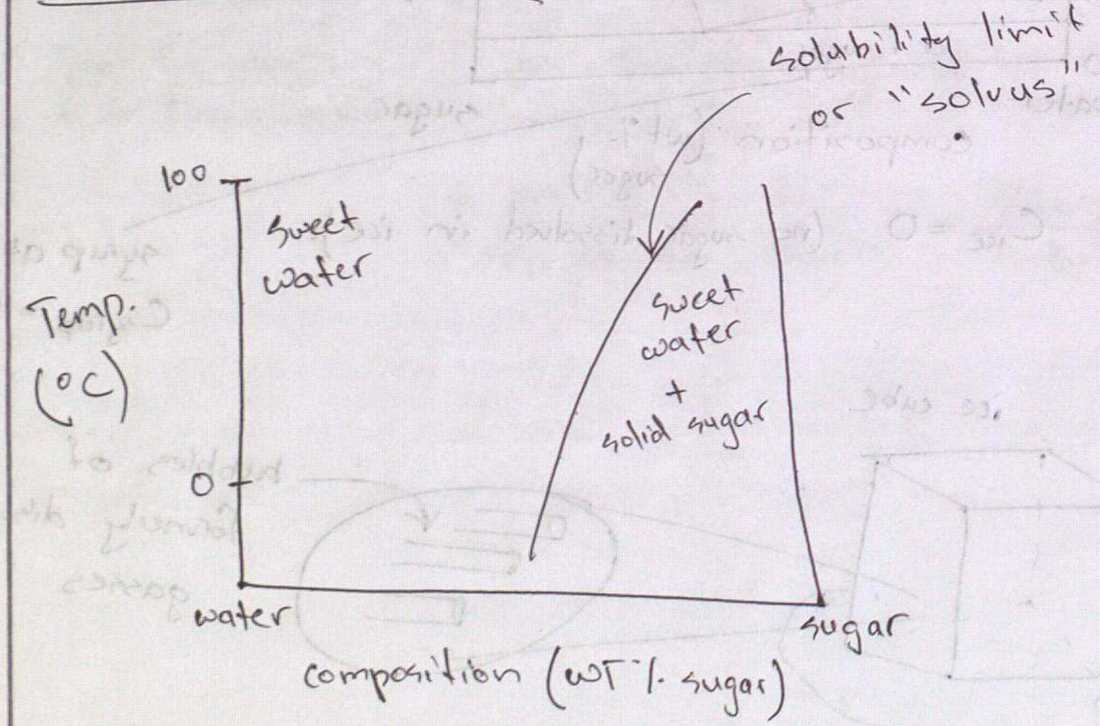
Ch.11 / Lec 31

The temperature Axis



one component only (water) so called ~~uniaxial~~ unary phase diagram

The composition



Ch.12

Phases

- * phase: a part of the system we are looking at that looks and behaves the same way

ex: add sugar to water → forms single phase (sweet water)

ex: add sand to water → forms 2 phases: 1) liquid H_2O 2) solid sand

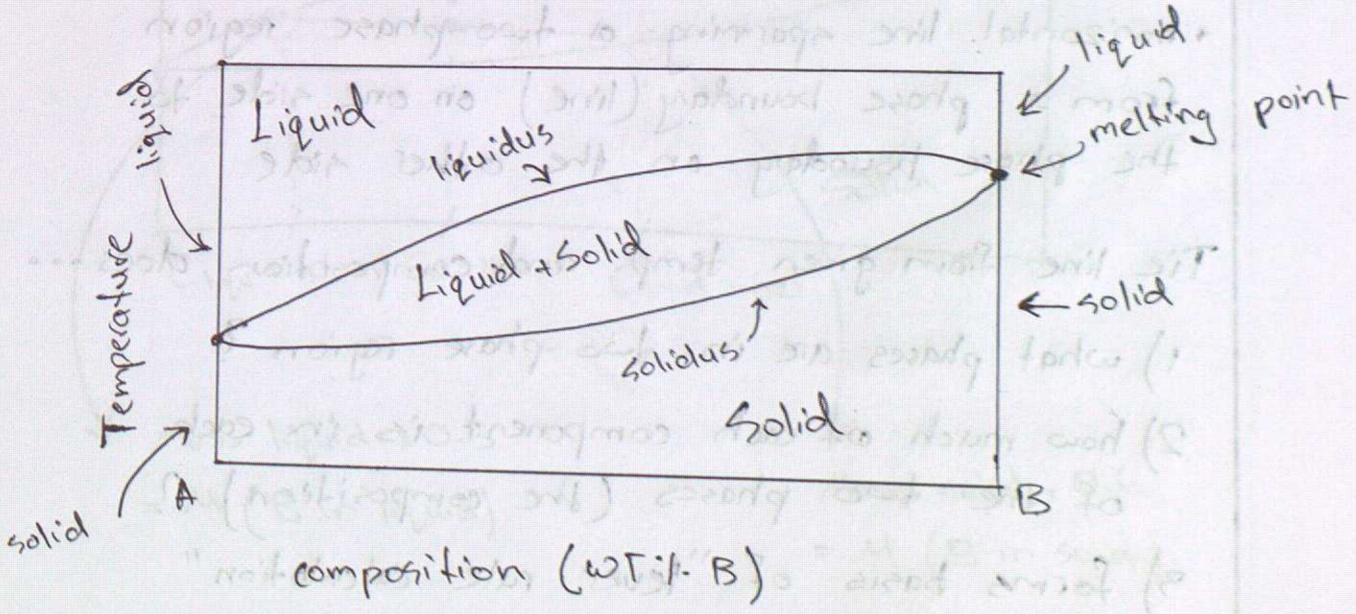
- * regions or fields: areas on phase diagram

Binary Phase Diagram

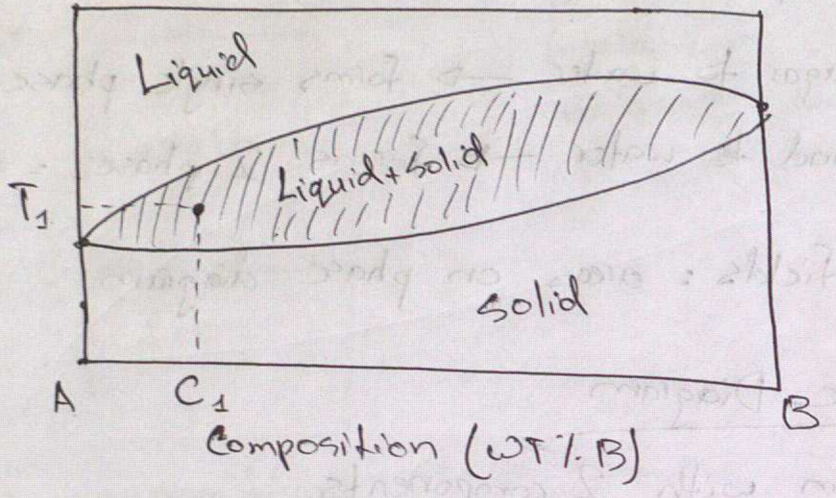
- * phase diagram with 2 components
- * unary → 1 component
- * binary → ~~3~~ 2 components

} * ternary → 3 components

- * isomorphous system: both components completely soluble in each other



Binary Phase Diagrams



- in "Liquid + Solid" region
  - ↳ two phases in equibrium (solid and liquid)
  - ↳ system "partly melted" or "partly solid"

The Tie Line

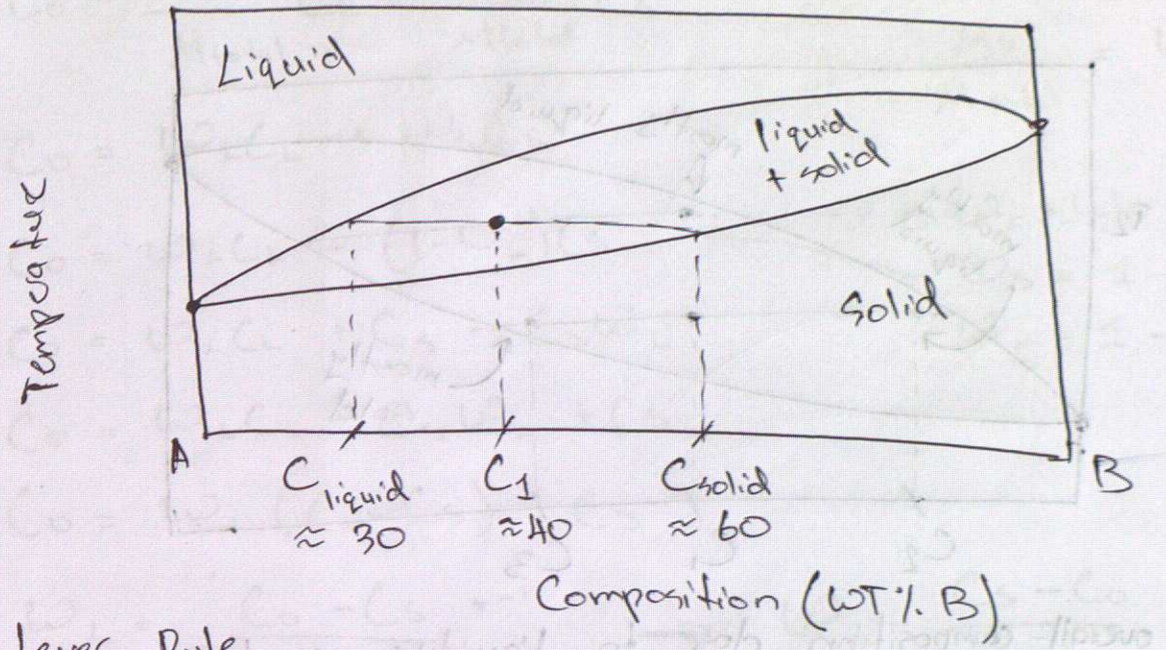
- horizontal line spanning a two-phase region from a phase boundary (line) on one side to the phase boundary on the other side

Tie line from given temp. and composition does...

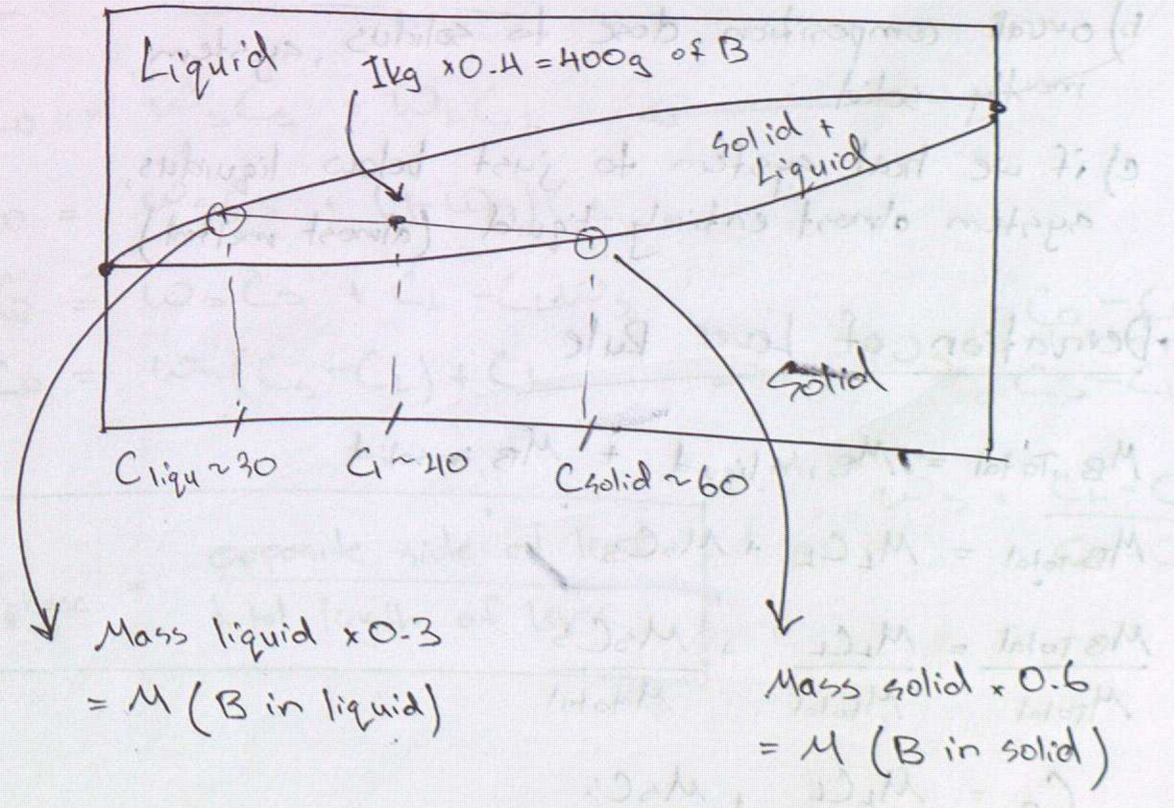
1) what phases are in two-phase region?
2) how much of each component is in each of the two phases (the composition)?
3) forms basis of "lever rule calculation"

Aug 19, 23

Tie Line



Lever Rule

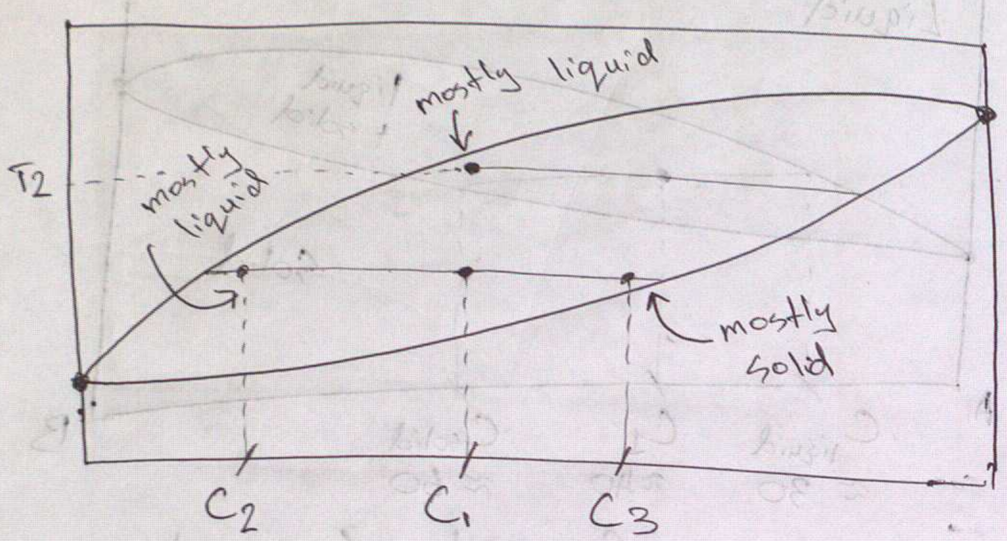


1kg × 0.4 = 400g of B

Mass liquid × 0.3 = M (B in liquid)

Mass solid × 0.6 = M (B in solid)

Mostly Liquid or Mostly solid?



a) overall composition close to liquidus, system mostly liquid

b) overall composition close to solidus, system mostly solid

c) if we heat system to just below liquidus, system almost entirely liquid (almost melted)

Derivation of Lever Rule

$$M_{B,Total} = M_{B,\text{in liquid}} + M_{B,\text{in solid}}$$

$$M_{B\,Total} = M_L C_L + M_S C_S$$

$$\frac{M_{B\,Total}}{M_{Total}} = \frac{M_L C_L}{M_{total}} + \frac{M_S C_S}{M_{total}}$$

$$C_0 = \frac{M_L C_L}{M_{total}} + \frac{M_S C_S}{M_{total}}$$

Lever Rule

$$C_0 = \frac{M_L}{M_{total}} C_L + \frac{M_S}{M_{total}} C_S$$

$$\frac{M_L}{M_{total}} = \omega_L$$

$$\frac{M_S}{M_{total}} = \omega_S$$

$$C_0 = \omega_L C_L + \omega_S C_S$$

$$\omega_L + \omega_S = 1$$
$$\omega_S = 1 - \omega_L$$
$$\omega_L = 1 - \omega_S$$

$$C_0 = \omega_L C_L + (1-\omega_L) C_S$$

$$C_0 = \omega_L C_L + C_S - C_S \omega_L$$

$$C_0 = \omega_L C_L - C_S \omega_L + C_S$$

$$C_0 = \omega_L (C_L - C_S) + C_S$$

$$\omega_L = \frac{C_0 - C_S \;{}^{\times -1}}{C_L - C_S \;{}^{\times -1}} \Longrightarrow \omega_L = \frac{C_S - C_0}{C_S - C_L}$$

$$C_0 = \omega_S C_S + \omega_L C_L$$

$$C_0 = \omega_S C_S + (1-\omega_S) C_L$$

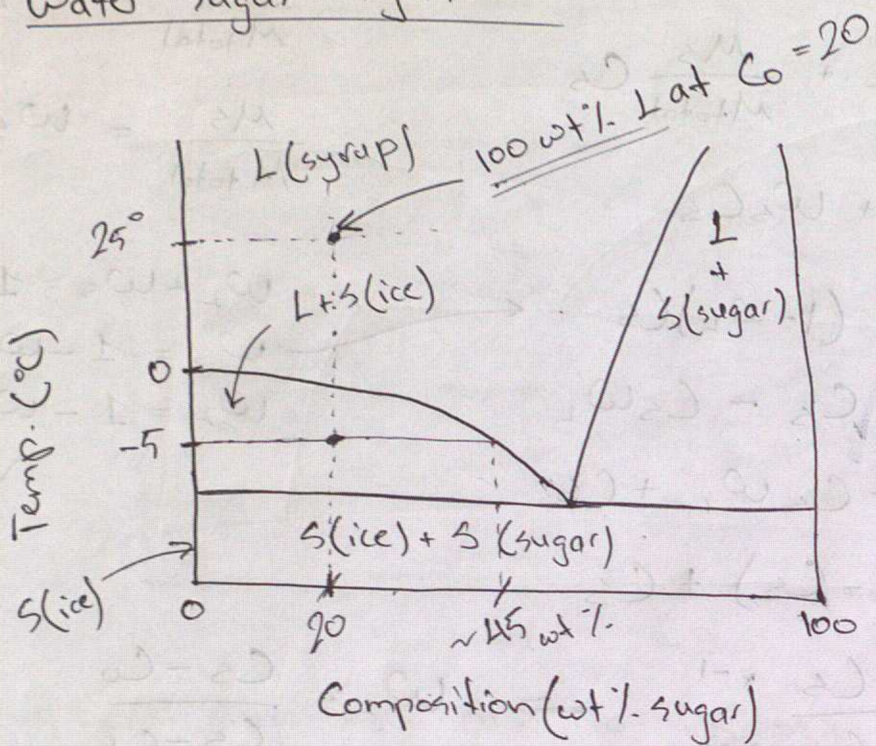
$$C_0 = \omega_S C_S + C_L - C_L \omega_S$$

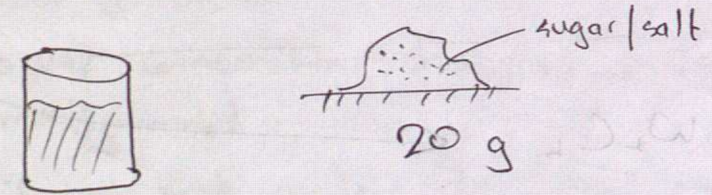
$$C_0 = \omega_S (C_S - C_L) + C_L \Longrightarrow \omega_S = \frac{C_0 - C_L \;{}^{\times -1}}{C_S - C_L \;{}^{\times -1}}$$

$$\omega_S = \frac{C_L - C_0}{C_L - C_S}$$

$$\boxed{\omega_{phase} = \frac{\text{opposite side of lever}}{\text{total length of lever}}}$$

Water Sugar System





80 g of water

C_0 = overall composition

$$= \frac{20g}{80+20} = 20 \text{ wt\%}$$

↓ cooled to -5°C

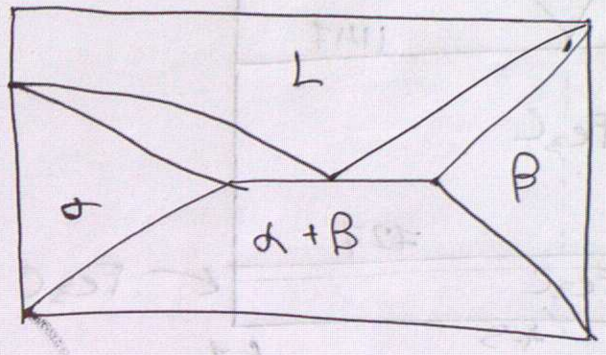
L @ C_L and S @ C_S

liquid at C_L = 45%wt

solid at C_S = 0 wt%

Binary Eutectic Phase Diagram

- system has one specific melting point that is below the melting point of each of its components

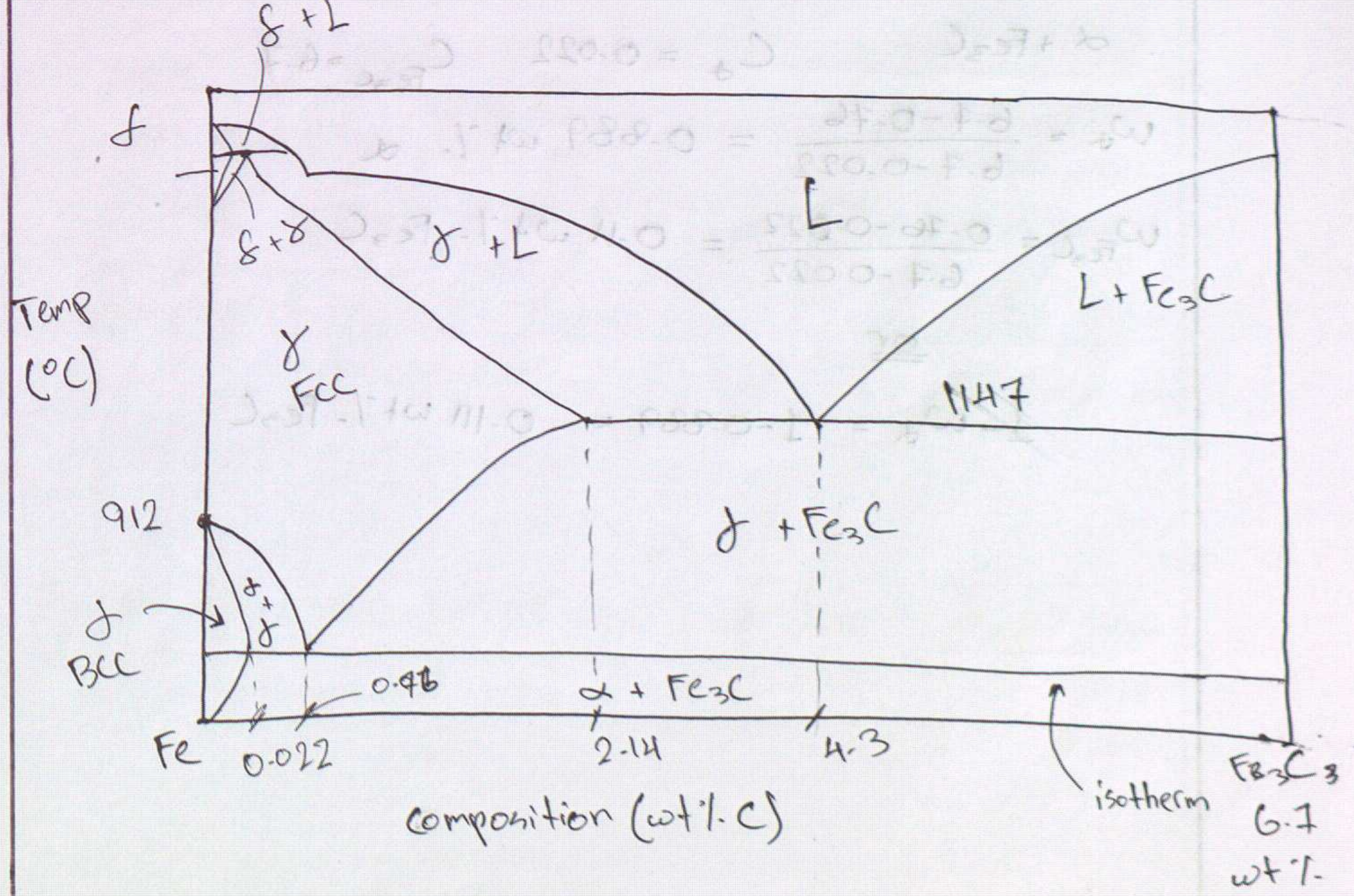


solid phases: lowercase greek letters

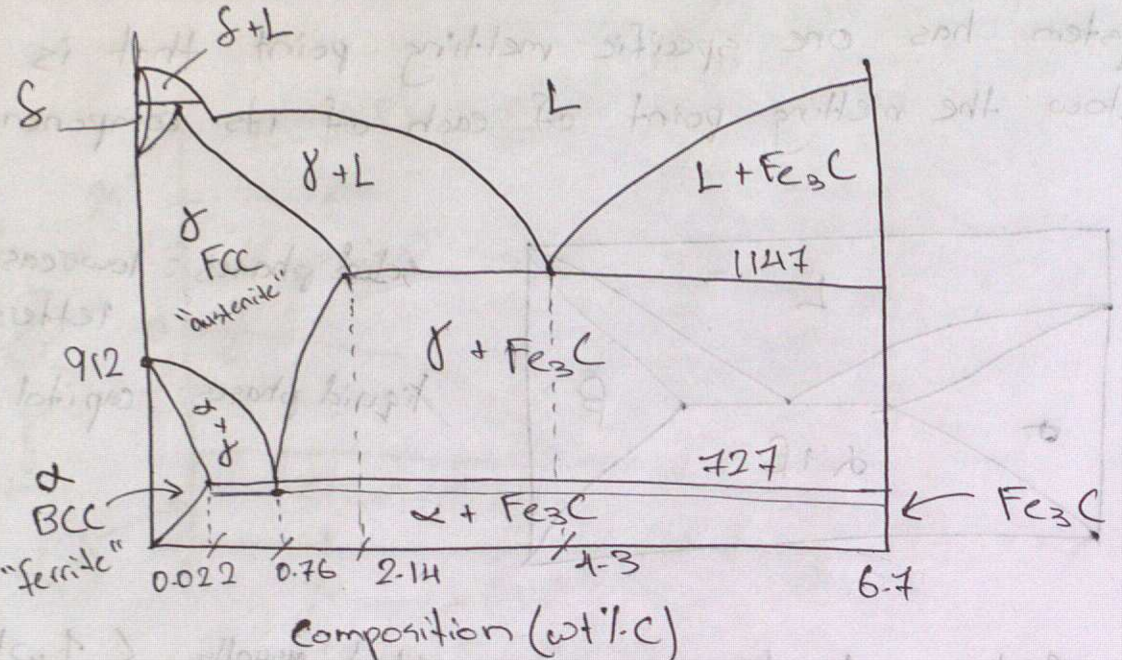
liquid phases: capital L

Iron-Carbon System

steel usually < 1 wt%



Iron-Carbon System



ex 0.76 wt% C steel (eutectoid steel) @ 726°C

$\alpha + Fe_3C$ $\quad C_\alpha = 0.022 \quad C_{Fe_3C} = 6.7$

$$W_\alpha = \frac{6.7-0.76}{6.7-0.022} = 0.889 \text{ wt\% } \alpha$$

$$W_{Fe_3C} = \frac{0.76-0.022}{6.7-0.022} = 0.11 \text{ wt\% } Fe_3C$$

or

$$1-W_\alpha = 1-0.889 = 0.111 \text{ wt\% } Fe_3C$$

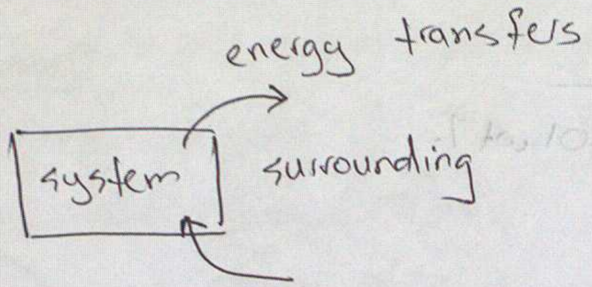
Q.12.4.1

C @ 0.01 wt%

Week 10 : Lec # 3

Thermodynamics

energy in the universe

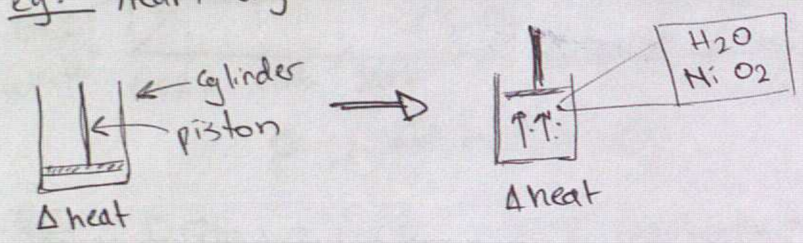


1st Law:

2nd Law: direction of energy transfer

3rd Law:

eg: steam engine



Internal Energy

- rotation energy
- vibration mobility
- molecular bonding energy

State Function: we can't meaure actual quantity, but we can measure change in quantity

↳ only dependent on state change

↳ how we got to the state doesn't matter

State Function

*Internal energy

Path Function : cares about path tavelled from initial state to final state

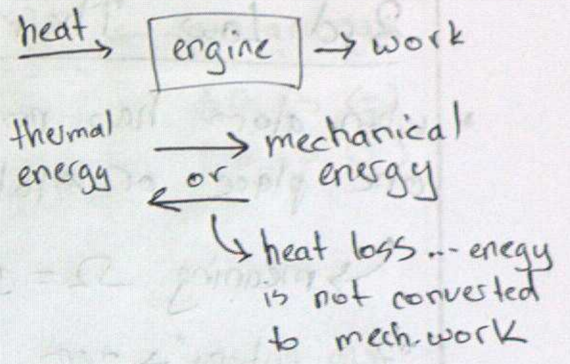
- heat
- work

Week 11: Lecture #2

Nov 29, 2023

1st Law Thermodynamics

* law of energy conservation
* not creating /destroying energy, only transforming from 1 form to another.



2nd Law Thermodynamics

* During spontaneous process, the total entropy change for the system and surrounding is positive

$$\Delta S = (\Delta S_{system} + \Delta S_{surrounding}) \geq 0$$

↑ $\Delta S_{universe}$

Definition

$$\boxed{S = \frac{q}{T}}$$

heat

temp.

* Entropy: measure of the number of ways of energy distribution

↳ measure of uncertainty of the precise levels of energy that are held by atoms

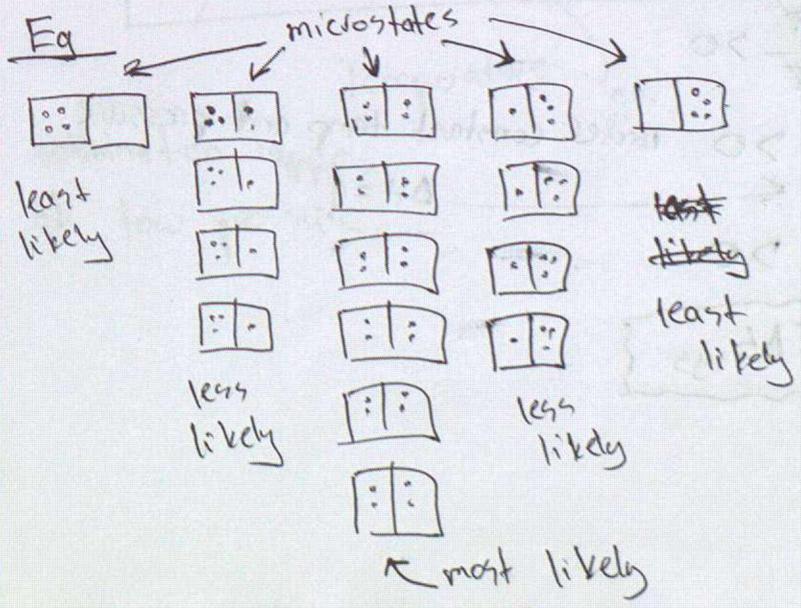
↳ measures disorder or randomness of the system

disorder ↑ spatial, thermal energy location.

randomness ← the number of possible arrangements

arrangements → microstate

Eg



$$S = K_B \ln \Omega$$

↑ Boltzmann Constant

↖ microstates

3rd Law Thermodynamics

- when atom has no thermal energy, they are in one place or state … microstate

↳ meaning $\Omega = 1 \longrightarrow S = k_B \ln \Omega$

$= k_B \ln(1)$

"zero entropy" → zero uncertainty about state of atom ← $\boxed{S = 0}$

- The entropy of a pure crystal will approach 0 as temperature approaches 0 kelvin.

Gibbs Free Energy

$$\boxed{\Delta G = \Delta H_{sys} - T\Delta S_{sys}}$$

we know $\Delta H = \Delta U + P\Delta V$

$\Delta S_{sys} + \Delta S_{surr} > 0$ for spontaneous processes

$\Delta S_{sys} - \frac{q}{T} > 0$ … multip. both sides by temperature

$T\Delta S_{sys} - \frac{q\cancel{T}}{\cancel{T}} > 0$

$T\Delta S_{sys} - q > 0$ under constant temp and pressure

$\xleftarrow{\quad} \Delta H = q$

$T\Delta S_{sys} - \Delta H > 0$

$$\boxed{\Delta G = \Delta H_{sys} - T\Delta S_{sys}}$$

Week 11: Lec. #3

$\Delta G = \Delta H_{sys} - T\Delta S_{sys}$

↑ Gibb's Free Energy

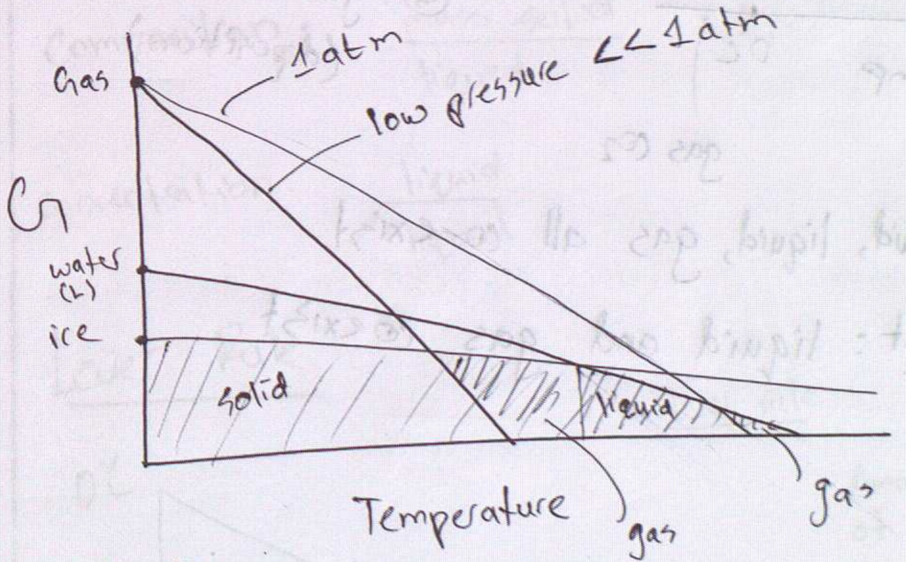
$\frac{\Delta G < 0}{\Delta S > 0}$ ← spontaneous

ΔG is (-)

ΔS is (+)

	$\Delta H < 0$ (exothermic)	$\Delta H > 0$ (endothermic)
$\Delta S > 0$	Spontaneous (All Conditions)	Spontaneous only at HIGH TEMP
$\Delta S < 0$	Spontaneous only at LOW TEMP (eg: water freezing)	Not Spontaneous (All conditions) … never spontaneous

(eg: water melting)



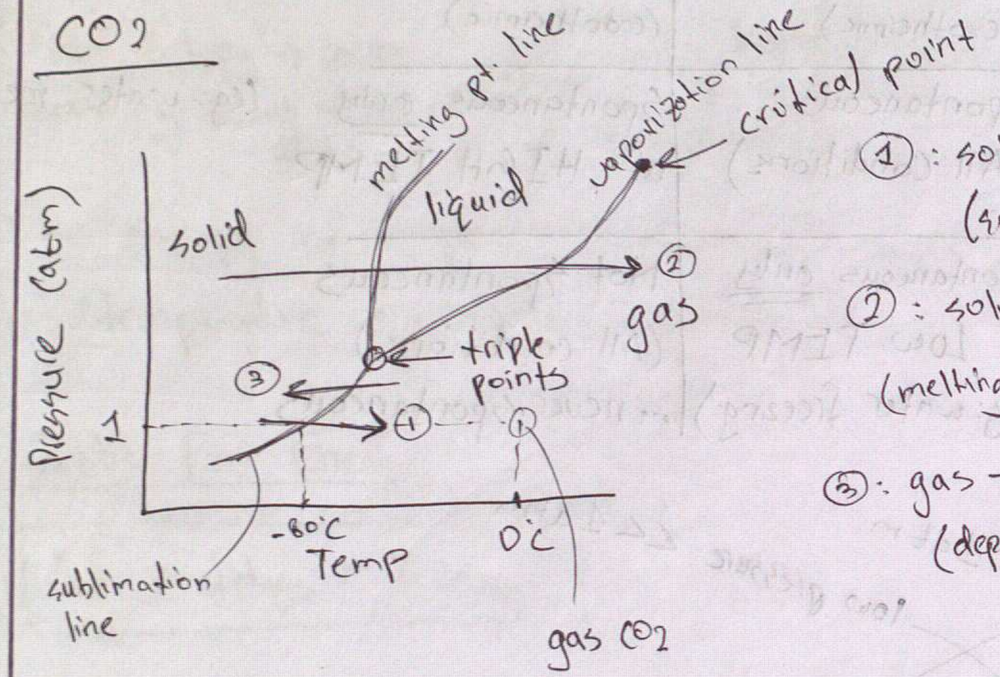
- sublimation happens at low pressure

Week 12: lec #1

Phase Diagram

- solid, liquid, gas
- w.r.t. temp and pressure

CO2



① : solid → gas
(sublimation)

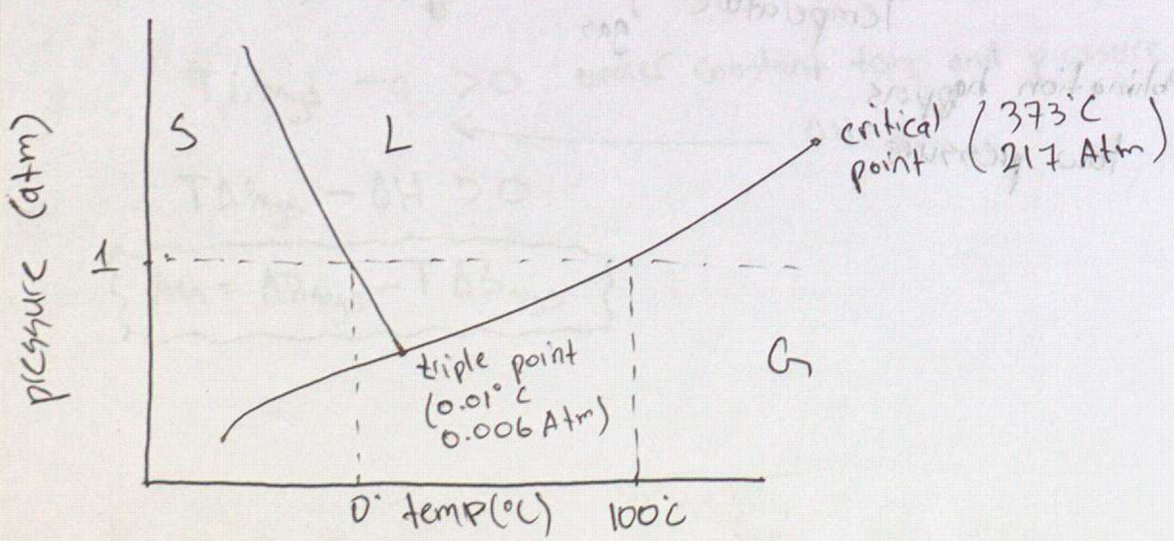
② : solid → liquid → gas
(melting) (vaporization)

③ : gas → solid
(deposition)

*<u>triple point</u>: solid, liquid, gas all co-exist

*<u>the critical point</u>: liquid and gas coexist

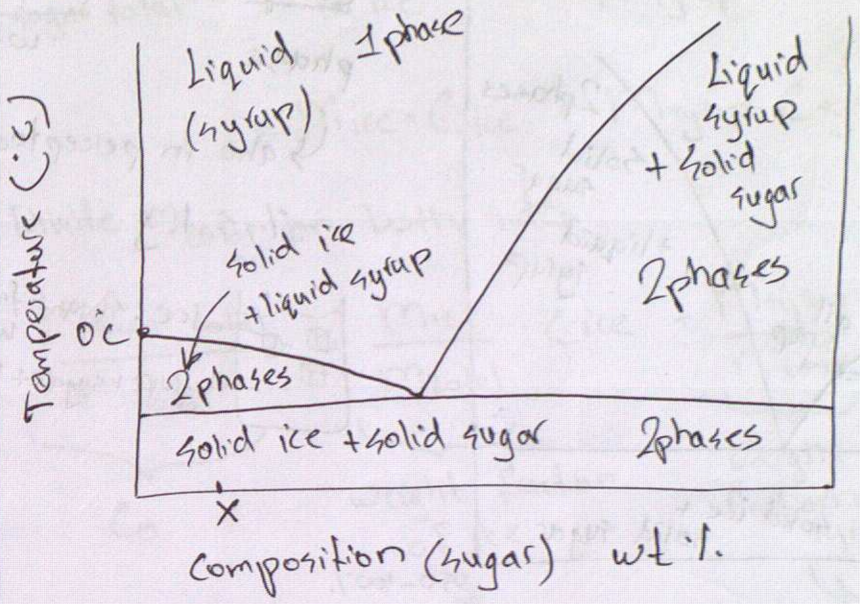
H_2O



Multicomponent Phase Diagram

eg: add sugar to water

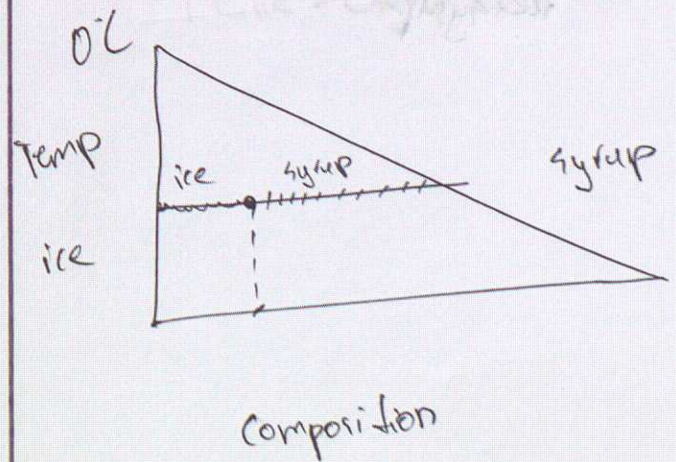
*assuming constant pressure



Composition : $\frac{\text{mass solid}}{\text{liquid}}$ wt%

concentration : $\frac{\text{liquid}}{\text{liquid}}$

Lever Rule



<u>lever rule</u>

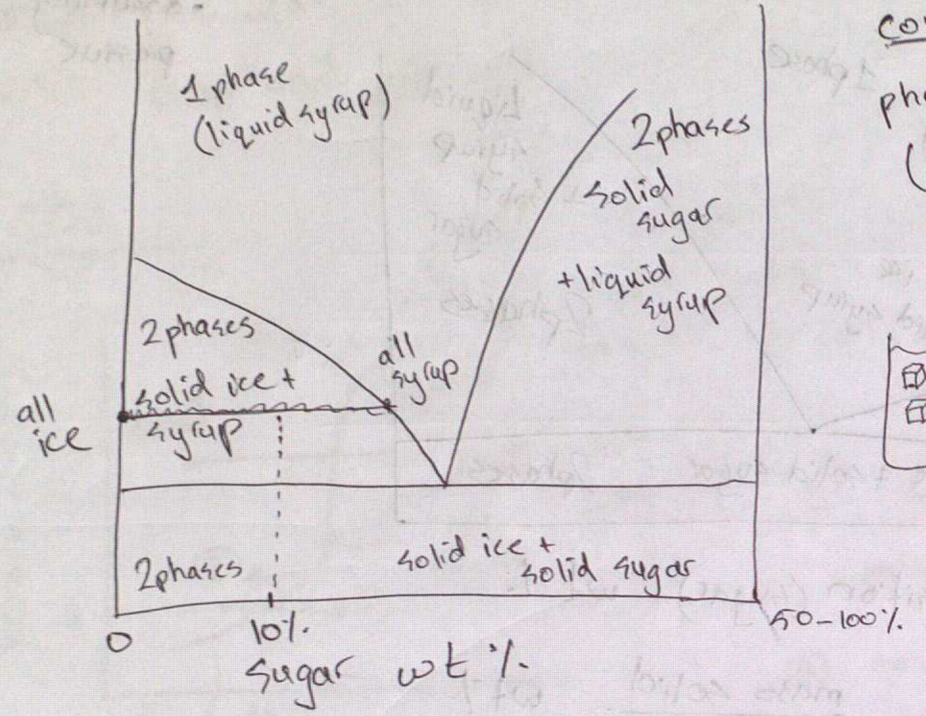
Amount of = $\frac{\text{opposite side of lever}}{\text{total lever length}}$

Amount of Ice = $\frac{\text{syrup}}{\text{ice + syrup}}$

Amount of syrup = $\frac{\text{ice}}{\text{ice + syrup}}$

Week 12: Lecture #12

Sugar + H_2O



2 Variables

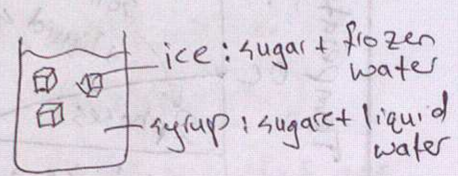
composition (component)

wt %

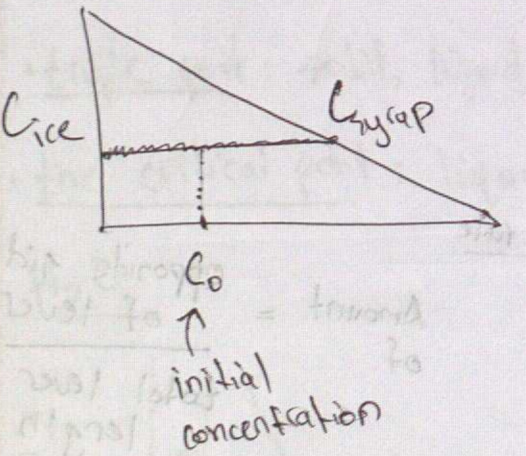
phase

↳ also in perceptage

% s, l, g



Say we have 10% sugar composition



$$\text{syrup phase} = \frac{\text{ice}}{\text{syrup}+\text{ice}}$$

$$\text{ice} = \frac{\text{syrup}}{\text{ice}+\text{syrup}}$$

Proof of Lever Rule

$$\text{Mass sugar total} = M_{\text{sugar in ice}} + M_{\text{sugar in syrup}}$$

composition

$$= M_{ice} \cdot C_{ice} + M_{syrup} \cdot C_{syrup}$$

Divide m_{total} on both sides

$$\underbrace{\frac{M_{\text{sugar total}}}{m_{total}}}_{C_0} = \underbrace{\frac{M_{ice}}{m_{total}}}_{\text{weight fraction of ice}} \cdot C_{ice} + \underbrace{\frac{M_{syrup}}{m_{total}}}_{\text{weight fraction of syrup}} \cdot C_{syrup}$$

weight fraction of ice ↓ W_{ice}

weight fraction of syrup ↳ W_{syrup}

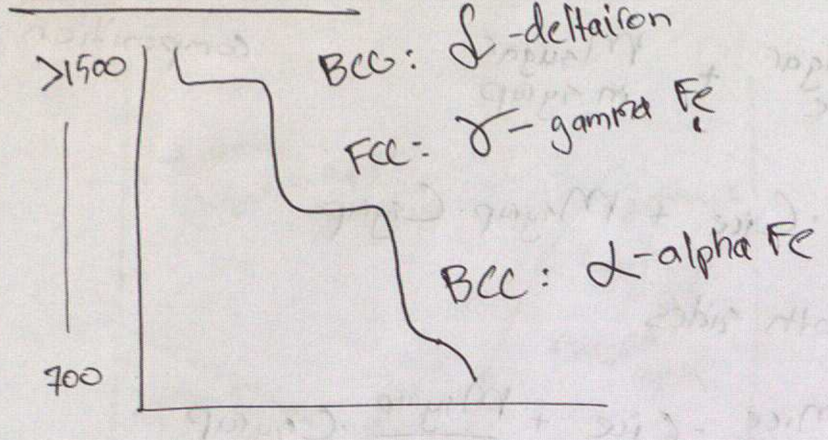
We know $W_{ice} + W_{syrup} = 1$

↳ $W_{syrup} = 1 - W_{ice}$ → substitute

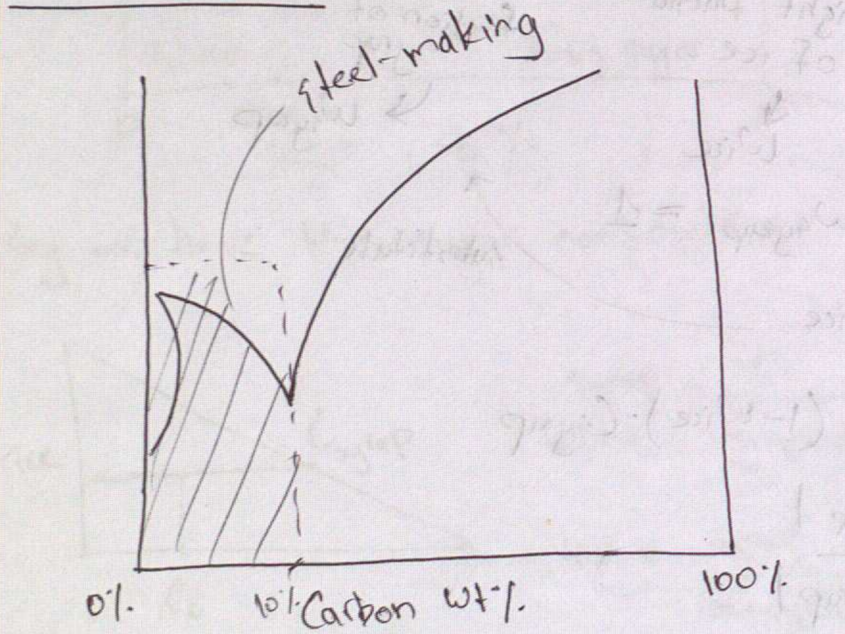
$$C_0 = W_{ice} \cdot C_{ice} + (1 - W_{ice}) \cdot C_{syrup}$$

$$W_{ice} = \frac{|C_0 - C_{syrup}|}{|C_{ice} - C_{syrup}|}$$

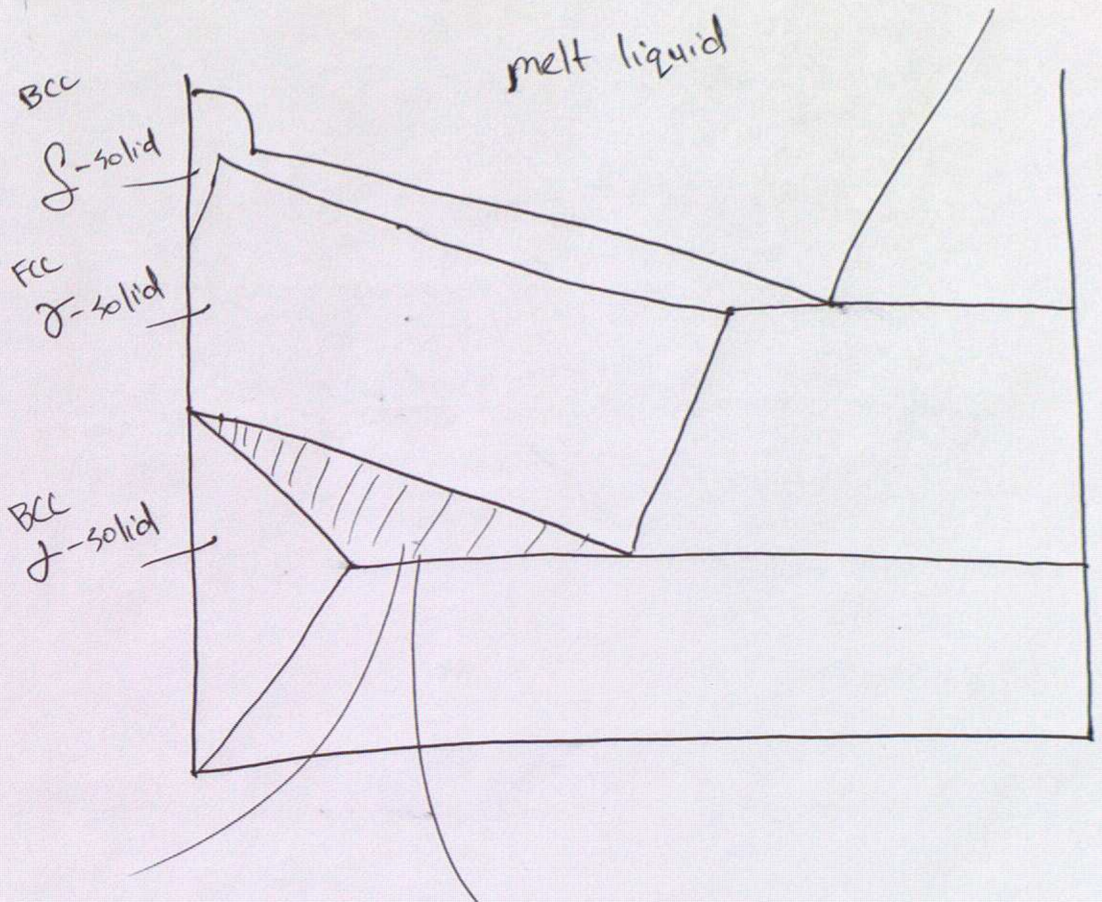
Fe: Iron Phases

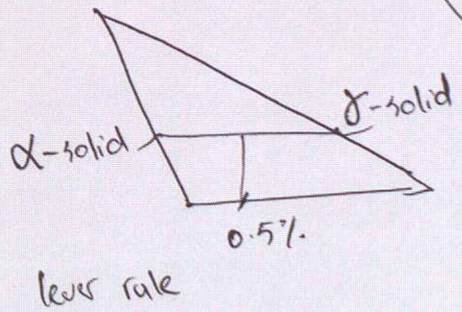


Steel: Fe + C



Iron-Carbide Phase Diagram





lever rule