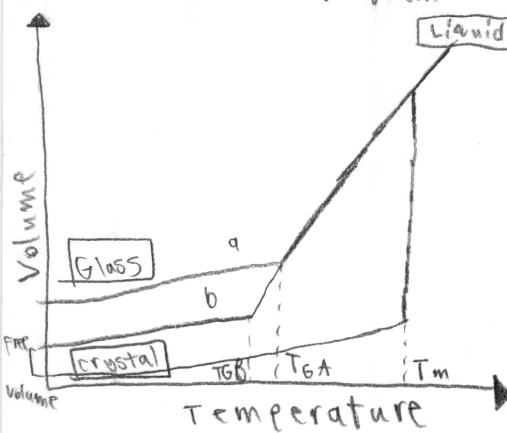


## Amorphous Solids

### Glass Transition Diagram



\* The faster the Glass cools  
or the more network  
modifiers added

### Long vs. Short Range Bonding Order

↳ Crystalline Materials have  
long range bonding order

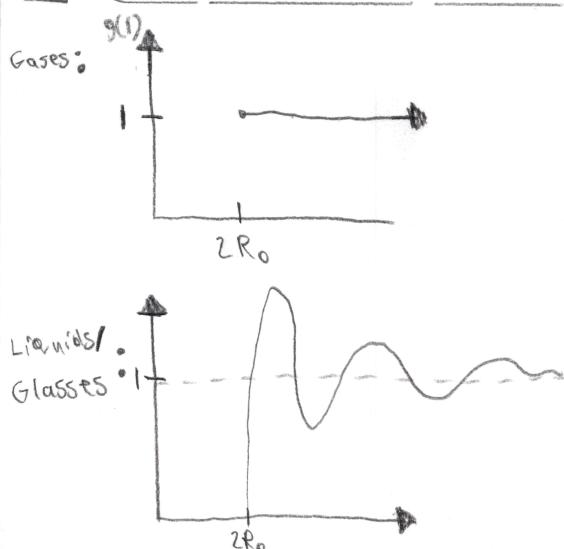
- Amorphous Materials have  
short range bonding order

### Two Descriptors

#### 1. Free Volume

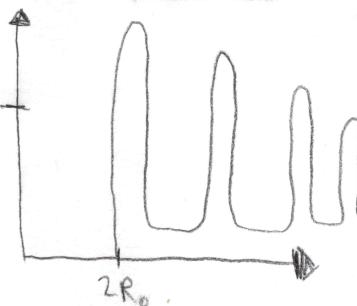
↳ Free Volume = (Volume of Amorphous  
Glassy State) - (Volume of  
Crystal State)

#### 2. Pair Distribution Function



## Structure

For Highly ordered,  
crystals



\* largest peak associated  
with # of nearest  
neighbors

\* Addition of Network  
Modifiers lowers  
Glass transition temp

### Random-Walk Model

$$R_0 = l\sqrt{n}$$

### For Volume scaling multiplier

$$\nu = 1/3 \quad \gamma = 3/5$$

$$n^{\nu} \quad n^{3/5}$$

$$n = \# \text{ of monomers}$$

### Tacticity

Isotactic - R groups on  
same side of  
Chain

Syndiotactic - R groups on  
Alternating  
sides of chain

Atactic - R groups Randomly  
Placed

### Crystallography

• Defined by Basis Vectors

$$\underline{t}_1 \ 8 \ \underline{t}_2$$

• Repeat distance is lattice  
constant

$$\text{in 3D volume} = |\vec{t}_1 \cdot \vec{t}_2 \times \vec{t}_3|$$

### Reciprocal Space

#### In 2D

- Given Regular Basis Vectors  $\vec{t}_1, 8\vec{t}_2$
- $R = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$

$$\vec{t}_1^* = \frac{R \vec{t}_2}{\vec{t}_1 \cdot R \vec{t}_2}$$

$$\vec{t}_2^* = \frac{R \vec{t}_1}{\vec{t}_2 \cdot R \vec{t}_1}$$

~~91090 + 231322~~

~~3245~~

~~91090 + 231322~~

~~27847 201781~~

~~(1-2) = 9 \*~~

~~$\frac{78}{78+9} = \frac{7}{17}$~~

~~$\frac{78}{78+9} = \frac{7}{17}$~~

~~91090 + 231322~~

~~27847 201781~~

~~100000 - 91090~~

~~98910 - 231322~~

~~75778 - 201781~~

~~15607 - 100000~~

~~5607 - 231322~~

~~5607 - 201781~~

~~5607 - 100000~~

~~5607 - 91090~~

~~5607 - 231322~~

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## 3D - Reciprocal Lattices

Given Lattice Vectors  $a_1, a_2, a_3$

$$a_1^* = \frac{a_2 \times a_3}{a_1 \cdot (a_2 \times a_3)}$$

$$a_2^* = \frac{a_1 \times a_3}{a_2 \cdot (a_1 \times a_3)}$$

$$a_3^* = \frac{a_1 \times a_2}{a_3 \cdot (a_1 \times a_2)}$$

Properties

1.  $\vec{g}_{hkl}$  is  $\perp$  to real space planes  $(hkl)$

2.  $|\vec{g}_{hkl}| = \frac{1}{d_{hkl}}$

Proof of 1.

$$\vec{g}_{hkl} = h\vec{a}_1^* + k\vec{a}_2^* + l\vec{a}_3^*$$

$$\vec{g}_{hkl} \cdot \vec{AB} = (h\vec{a}_1^* + k\vec{a}_2^* + l\vec{a}_3^*) \cdot \left( \frac{\vec{a}_1}{h} + \frac{\vec{a}_2}{k} \right)$$

$$= h - k = 0 \quad \text{which means } \perp$$

Proof of 2.

$$|\vec{a}_3^*| = \frac{1}{a_3 \cdot (\vec{a}_1 \times \vec{a}_2)} = \frac{1}{d \text{ (Plane spacing)}}$$

### Bragg's Law

$$2d \sin(\theta) = n\lambda$$

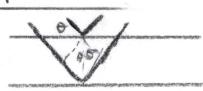
$d$  = interplanar spacing

$\lambda$  = wavelength of radiation

$n$  = an integer (usually 1)

$\theta$  = Bragg's Angle

Proof:



$\{ d \}$  For constructive interference to occur  
 $2d \sin(\theta)$  must equal  
 Integer multiple of wavelength

### Lau's Condition + STRUCTURE FACTOR

$$F(\Delta k) = \sum_{k=1}^N f(r_k) e^{2\pi i (\Delta k \cdot r)}$$

↳ We get constructive interference when  $\Delta k$  is reciprocal lattice vector

### Structure Factor

$$F(\Delta k) = \sum_{n=1}^N f(r_n) e^{2\pi i (hxt+kyt+lzt)}$$

## STRUCTURE

where

$N$  = # of atoms in motif  
 $f$  = specific structure factor of atom

$(hkl)$  = Plane being observed

$(x,y,z)$  = Positions of atoms

Positions of atoms in common structure

SC:  $(0,0,0)$

BCC:  $(0,0,0), (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

FCC:  $(0,0,0), (\frac{1}{2}, \frac{1}{2}, 0), (0, \frac{1}{2}, \frac{1}{2}), (\frac{1}{2}, 0, \frac{1}{2})$

### Selection Rules

SC: Any  $h, k, l$

BCC:  $(h+k+l)$  must be even

FCC:  $h, k, l$  must all be Even or Odd

### 14 Bravais Lattices

Triclinic	$a_1 \neq a_2 \neq a_3$ $a_{12} \neq a_{23} \neq a_{13}$
Monoclinic (+1 Volume centers)	$a_1 \neq a_2 \neq a_3$ $a_{23} = a_{13} = 90^\circ, a_{12} \neq 90^\circ$
Orthorhombic +VC, FCC, B <sub>cc</sub> , B <sub>sr</sub> center	$a_1 \neq a_2 \neq a_3$ All angles $90^\circ$
Tetragonal +VC	$a_1 = a_2 \neq a_3$ All angles $90^\circ$
Trigonal	$a_1 = a_2 = a_3$ $a_{12} = a_{13} = a_{23} < 120^\circ$
Cubic	$a_1 = a_2 = a_3$ All angles $90^\circ$
Hexagonal	$a_1 = a_2 \neq a_3$ $a_{12} = 120^\circ$ $a_{23} = a_{13} = 90^\circ$

### Combination Theorem #1

If there exists an Angled Rotation & Mirror Plane, there must be another mirror plane ~~passing at angle A/2~~

angle A/2

### Combination Theorem #2

If there are 2 Rotation Vectors separated by translational vector  $t$ , there exists another angular rotation distance D above midway point

$$D = \frac{t}{2} \cot\left(\frac{d}{2}\right) \quad t = \text{translation vector}$$

$$d = \text{Rotation angle}$$

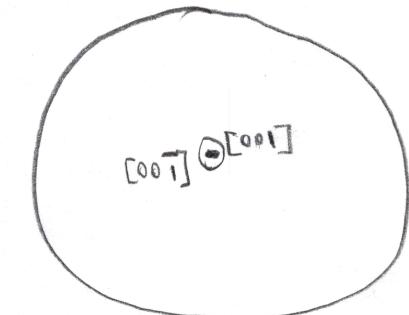
### Combination Theorem #3

$m \quad m'$   $m$  • A combo of a mirror Plane & Translation creates a new mirror plane

### Stereo graphic projection

○ - Above Equatorial Plane

○ - Below Equatorial Plane



### TENSORS

Response = Property • Stimulus

### Ex. Conductivity

$$J = \sigma \cdot E$$



$$\sigma_{ij} = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{pmatrix}$$

Simplifying constraint  $\sigma_{ij} = \sigma_{ji}$   $9 \rightarrow 6$

### IN 2D

For Rectangles:  $\begin{pmatrix} \sigma_{11} & 0 \\ 0 & \sigma_{22} \end{pmatrix}$

For Squares:  $\begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix}$

### Transforming Tensors

$$T'_{ij} = L \cdot T \cdot L^{-1}$$

(transformed tensor)

original tensor

inverse of Transform Matrix



## Quasi Crystals

- Quasi-Periodic Crystals have no translational spacing
- The structure preserves long-range rotational symmetry but has no translational order

### Review

- Amorphous Materials possess Short Range Order but lack long range order

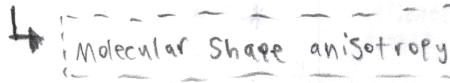
- Long range positional order  
 Long range orientational order

Plastic Crystals have long range translation but no long range orientation

### Liquid Crystal

- Crystals that lack long-range translational order, But possess Long-Range Orientation are called Liquid Crystals

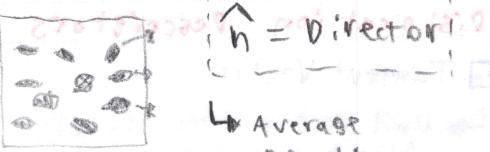
\* Key structural requirement for Liquid Crystals



- Calamitic → Rod-Shaped
- Diskotic - Disk Shape
- Cholesteric - Bent Shape

### Director

- The director is the preferred axis of LC Molecule orientation



↳ Average Direction

## Structure 3

### Nematic Liquid Crystal

- No Positional order
  - Long Range orientational order
- ↳ Typically composed of Rod-Like Molecules



### Chiral Nematic Liquid Crystal

- Only applies for Chiral (Bent) Molecules
- There will be a preferential twist in this liquid crystal



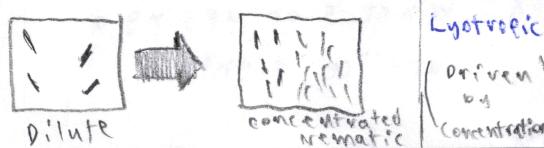
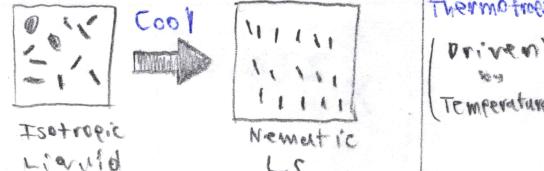
- The director  $\hat{n}$  changes & rotates as molecules do

### Smectic Liquid Crystal

- There are Planar Arrangements of Liquid Crystal Molecules

NOTE: This is more ordered than the Nematic Phase

### Thermotropic & Lyotropic LC



### Ordering Summary

	Positional order	Orientational order
Solid Crystal	✓	✓
Plastic Crystal	✓	✗
Liquid Crystal	✗	✓
Isotropic Liquid	✗	✗

### Descriptors of Liquid Crystal

#### 1. Orientational Parameter S

#### 2. Translational Parameter $\Sigma$

#### 3. PDF

#### Orientational Order Parameter $S$

- For Perfect crystal  $\theta = 0^\circ$   
For Isotropic liquid  $\theta = \text{Random}$

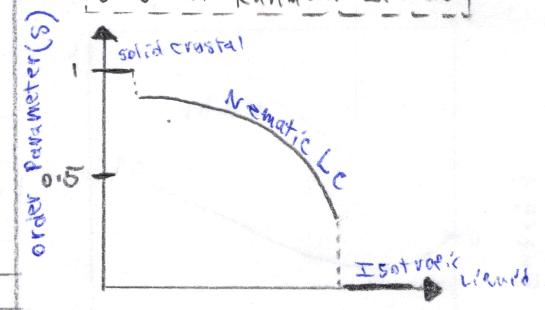
$$S = 2 \langle \cos^2 \theta \rangle - 1$$

↳

$$\cos^2(\theta) = \frac{\int_0^{\pi} \cos^2 \theta p(\theta) d\theta}{\int_0^{\pi} p(\theta) d\theta}$$

$S=1$  for Perfect crystal

$S=0$  for Random Liquid



Temperature

#### Translational Order Parameter

$\Sigma$  =  $\frac{1}{a} \int_{-a/2}^{a/2} \cos\left(\frac{2\pi z}{a}\right) \cdot p(z) dz$

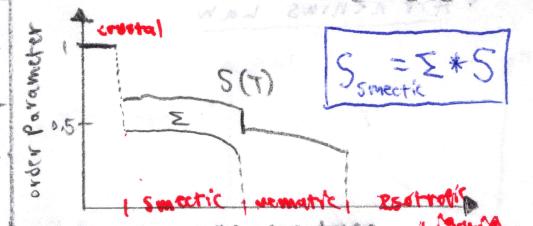
$a$  = Distance between layers  
 $p(z)$  = probability function of finding particle at distance  $z$

$$\Sigma = \int_{-a/2}^{a/2} p(z) dz$$

$$\Sigma = 0 \text{ for Nematic & Liquid }$$

$$\Sigma = (0-1) \text{ for Smectic LC }$$

$$\Sigma = 1 \text{ for Perfect + crystal }$$



PDF is to notes

• Crystalline Looking for smectic

• Amorphous Looking for Nematic

## Point Defects

- Some Defects can be in Equilibrium configuration
- ↳ b/c Gibbs Free Energy is minimized w/ defects

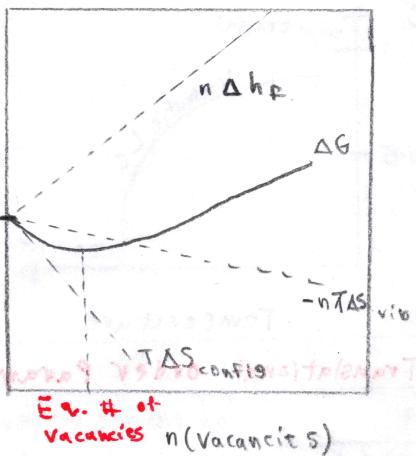
### Thermo Dynamics of Point Defects

$$\Delta G = \Delta H - T\Delta S$$

where

$$\Delta H = n * \Delta h_f$$

$$\Delta S = (\Delta S_{\text{vibration}} * n) + \Delta S_{\text{configuration}}$$



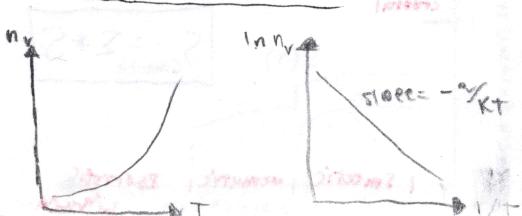
\* Entropy of Mixing is responsible for Spontaneous Existence of Defects

### Concentration of Point Defects

$$X_v = \frac{n}{n+N} \sim e^{\left(\frac{-q}{kT}\right)}$$

\* Important Assumption  $N > n$  & often we can assume  $N = \text{Avogadro's #}$

### Arrhenius Law



- In General Defect concentration increases w/ Temperature

Substitutions much more likely than Interstitials

### Solid Solutions

- Interstitials fill the voids & have a Much smaller Atomic Diameter than that they enter

conditions for Substitution:

1.  $\Delta$  Radius  $< 15\%$
2. Elements have similar Electro Negativity
3. Same Crystal Structure
4. The same preferred Valence state

### Frenkel & Schottky Defects

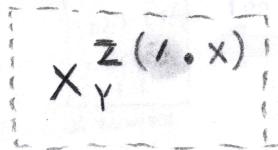
#### Frenkel Defect

↳ A Cation Vacancy / cation Interstitial Pair

#### Schottky Defect

↳ A paired set of cation-Anion Vacancies

### Kroger-Vink Notation



X = what is occupying a lattice site

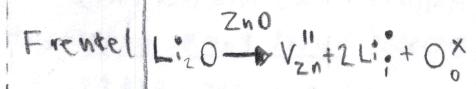
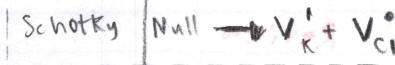
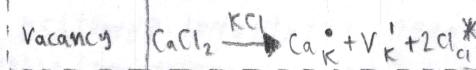
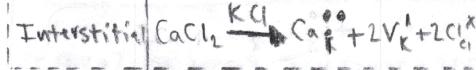
Y = what was occupying site Previously, or i for Interstitial

Z = Charge relative to what normally occupies site

X Y X

### \* Both Mass & Charge

Must be balanced



### Diffusion

Diffusion Co-efficient Determines

Kinetics & speed of diffusion

$$D = D_0 * e^{\lambda(-\alpha_d / kT)}$$

D = Diffusion Co-efficient

$D_0$  = Pre-Exponential Factor

$\alpha_d$  = Activation energy

R = gas constant

T = Absolute Temperature

\* Diffusion Driven by Difference in chemical Potential

### Tensile & Shear Stress

#### Tensile Stress



$$\sigma = F_T / A_0$$



$$\tau = F_S / A_0$$



### Dislocation Descriptors

#### Tangent Vector

↳ Unit vector that points along the direction of a defect

#### Burgers Vector

↳ Describes the closure failure of a circuit that encloses the dislocation

- Edge Dislocations have  $b \perp \tau$
  - Screw Dislocations have  $b \parallel \tau$
- Dislocation Motion, Slip Plane, & Direction**

- A dislocation moves along a Slip Plane in a Slip Direction (Must contain a Burgers vector  $\delta$  line vector)

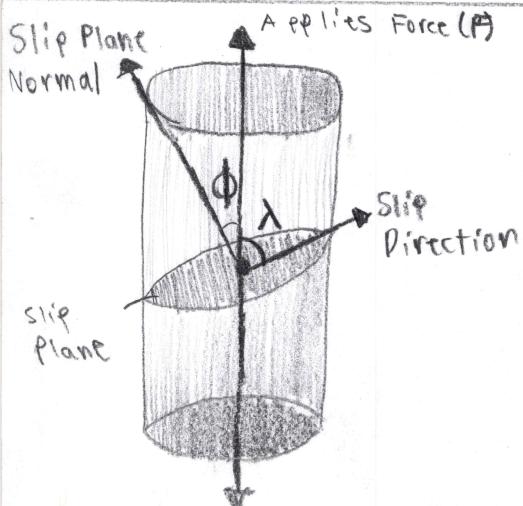
### Slip Plane

↳ Miller Planes with highest Planar Density

### Slip Direction

↳ Directions of Movement (Highest Linear Density) Along Slip Plane

### Resolved Shear Stress



$$T_r = \sigma \cos(\phi) \cos(\lambda)$$

$$\left( \begin{array}{l} \text{resolved} \\ \text{shear} \\ \text{stress} \end{array} \right) = \sigma \cos(\phi) \cos(\lambda)$$

Applied Tensile Stress

### Condition for Dislocation:

$$T_r > T_{\text{critical stress}}$$

### Strengthening Mechanisms

- Mechanical Resistance of a Crystal is Directly Related to the ease with which Dislocations are generated & Moved

### Methods:

#### 1. Reduce Grain Size

↳ This inhibits one-directional slippage

#### 2. Form Solid Solutions

↳ Impurities warp Lattice & make it more difficult for slip motion to occur

#### 3. Precipitate Hardening

↳ Introduction of entirely separate phase into material

### Surface Free Energy

- An interface is where the co-ordination # of a material is less than that of its bulk
- This gives rise to Excess Surface Energy per unit Area

### Wulff Shape

1. On a Wulff net, draw a group of vectors from the origin whose length is proportional to the surface tension of the crystal

2. Draw at the end of each vector a  $\perp$  plane

The shape enclosed is the Wulff shape

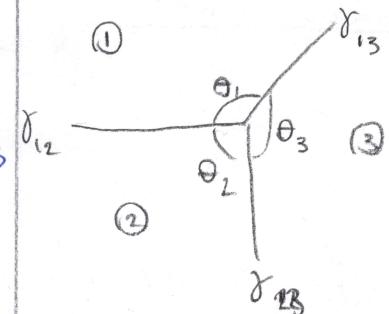
### Stacking Faults

"Perfect Dislocation"  $\rightarrow$  "2 Partial Dislocations"

### \*Grain Boundaries

- Case 3 Grains w/ different phases present

$$\frac{\gamma_{13}}{\sin \theta_2} = \frac{\gamma_{23}}{\sin \theta_1} = \frac{\gamma_{12}}{\sin \theta_3}$$



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$$(K)_{\text{exp}}(\phi)_{\text{exp}} = \begin{pmatrix} \text{horizontal} \\ \text{vertical} \end{pmatrix}$$

$$= \begin{pmatrix} \text{horizontal} \\ \text{vertical} \end{pmatrix}$$

## Defining the System

1. Open / Closed

2. Rigid / Non-Rigid

Implications: whether or not  $dV=0$  for work term

3. Adiabatic / Diathermal

Implications: whether or not a heat term exists ( $Q=C_p dT$ )

Compressibility & Thermal Expansion

$$\beta = -\frac{\partial \ln V}{\partial P}$$

useful:

$$\partial \ln V = -\beta \partial P$$

$$\left[ \ln \left( \frac{V_f}{V_i} \right) = -\beta (P_f - P_i) \right]$$

$$d = \frac{\partial \ln V}{\partial T} \Big|_P$$

useful:

$$\partial \ln V = d \partial T$$

$$\left[ \ln \left( \frac{V_f}{V_i} \right) = \alpha (T_f - T_i) \right]$$

Ideal Gas Law

$$PV = nRT$$

Intensive vs. Extensive

• Intensive = Can be defined at any point in system

• Extensive = Measurement requires aggregation

## Thermo

\*\* Process Classifications \*\*

isothermal = Fixed Temperature

Adiabatic = No heating across boundary

Iso Baric = Fixed Pressure

Isochoric = Fixed Volume, No work

Insulating = No Heating

Diathermal = Can exchange Heat over Boundary

Rigid = No change of Volume

calculating Q

$$Q = \int C_p \text{ or } C_v dT$$

First Law of Thermo

$$dU = \delta Q + PdV + H dN$$

2nd Law of Thermo

$$dS = \frac{\delta Q}{T} \quad \text{Only for Reversible Processes}$$

useful:

$$S = S_0 + \frac{C_p dT}{T} \Big|_{T_i}^{T_f}$$

\* Entropy For a Reversible Process is Always 0,

however you can use a reversible Pathway to Find Entropy

\* General Strategy \*

- Given Dependant Variable Z  $\geq 8$  Independent Variables  $\leq 8$  Y

Step 1 Write exact Differential

Step 2 Express in terms of differentials you know (dT, dP)

Step 3 Collect terms

Step 4 Solve 8

Evaluate to Get Co-efficients. Carry on with problem

\* CHOOSE Independent Variables Carefully

Such that you can Make one Drop Out!

- ## A p plications to Ideal Gas

## Ideal Gas

$$\bullet \text{ PV} = nRT$$

$$d = \frac{1}{T}$$

$$\beta = \frac{1}{p}$$

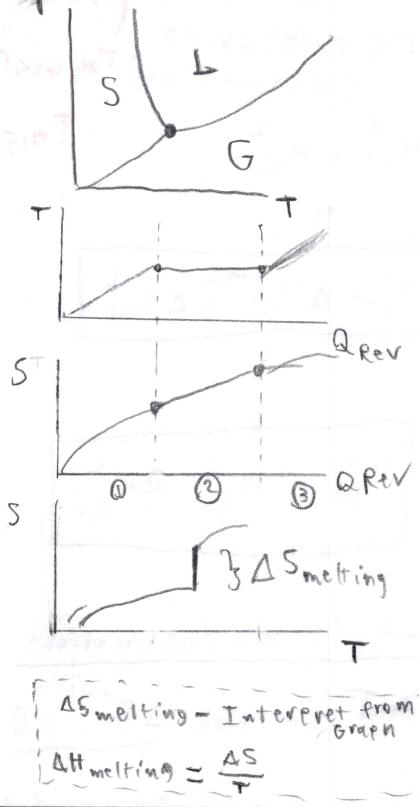
$$C_V = C_p - R$$

$$C_p = \frac{5}{2} R$$

$$\Delta V = \frac{3}{2} R (T_2 - T_1)$$

# Phase transitions

## Unary Phase Diagram



## Building Unary Phase Diagrams

$$dG = SdT + VdP + \mu dN$$

$$H = \left. \frac{\partial G}{\partial n} \right|_{T, P} \quad \begin{array}{l} \text{Molar Gibbs} \\ \text{Free energy} \end{array}$$

Proof that  $H$  is Molar Gibbs

$$G = \frac{G'}{n \text{ moles}} \quad \left\{ H = \frac{\partial G'}{\partial n} = \frac{\partial(nG)}{\partial n} = \boxed{G} \right.$$

Determining Equilibrium conditions

- At each  $(T, P)$  calculate  $H$  for all known phases
- Equilibrium is phase with lowest  $H$

If  $H_A = H_B = H_C$  phase coexistence occurs

Using initial known state

$$\int_i^f dH = - \int_i^f dTS + \int_i^f dPV$$

Clausius-Clapeyron

\* Useful for Vapor pressure

$$\frac{dP}{dT} = \frac{\Delta S}{\Delta V} = \frac{\Delta H}{T \Delta V} \quad \begin{array}{l} \text{Isothermal} \\ \text{transition only} \end{array}$$

## Therm O

### Proof of C-C

- On Co-existence line

$$H_A(T, P) = H_B(T, P)$$

$$dH_A(T, P) = dH_B(T, P)$$

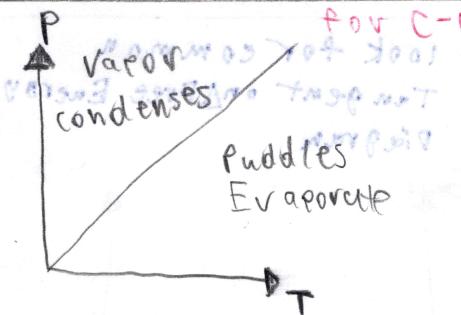
$$dH_A = -S_A^\alpha dT + V_A^\alpha dP$$

$$dH_B = -S_B^\beta dT + V_B^\beta dP$$

$$(S_A^\alpha - S_B^\beta) dT = (V_A^\alpha - V_B^\beta) dP$$

$$\frac{dT}{dP} = \frac{\Delta S_B - \Delta S_A}{\Delta V_B - \Delta V_A}$$

### Simplifying Assumptions



- On Co-existence Line

$$\boxed{P = P_{SAT}}$$

### For Condensed Phase

Vaporization we

make these key

assumptions

(1) Gasses Behave Ideally

$$(2) \Delta H(T, P) = \Delta H(T_0, P_0)$$

(3) Volume of Gas is

much larger than  
Solid or liquid

$$V_g \gg V_L, V_S$$

As a consequence

$$\frac{dP}{dT} = \frac{\Delta H(T_0, P_0)}{T_0 V_g}$$

$$\frac{dP}{dT} = \frac{\Delta H(T_0, P_0)}{T_0 \frac{nRT}{P}}$$

$$\frac{dP}{P} = \frac{\Delta H(T_0, P_0)}{T_0} dT \rightarrow \boxed{\text{solve}}$$

### Gibbs Phase Rule

\* Phases w/ lower densities usually preferred at higher pressures

### (1) Matrix of Variables

$$\left. \begin{array}{l} (T_1, P_1, X_1, X_2, \dots, X_{C-1})^\alpha \\ (T_2, P_2, X_1, X_2, \dots, X_{C-1})^\beta \\ \vdots \\ (T_p, P_p, X_1, X_2, \dots, X_{C-1})^{P_h} \end{array} \right\} \text{Ph}(c+1)$$

### (2) constraints from Equilibrium

$$\left. \begin{array}{l} T^\alpha = T^\beta = T^{P_h} \\ P^\alpha = P^\beta = P^{P_h} \\ H_1^\alpha = H_1^\beta = H_1^{P_h} \end{array} \right\} (c+2)(P_h-1)$$

Degrees of Freedom

$$= \text{Ph}(c+1) - (P_h-1)(c+2)$$

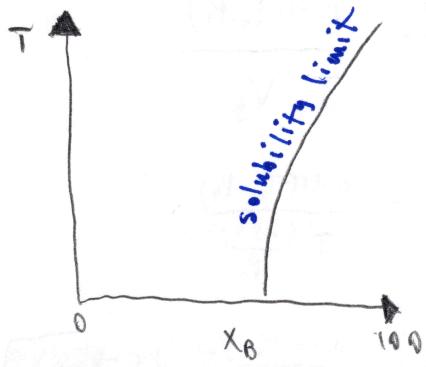
$$= \boxed{c+2 - P_h}$$

f = degrees of freedom

c = # of components

p = # of phases

## Binary Phase Diagrams



Solubility - Mol Fraction at which compound A starts showing in 2 phases of B

Eutectic point - Lowest temp at which 2 solid phases become one liquid phase

Eutectoid - Point at which 2 solid phases above certain temp become 1 solid phase

Peritectic point - Liquid + Solid phase become 1 solid phase

Peritectoid - 2 solid phases cool to form 1 solid phase

Line compound - Equilibrium phase that exists along a single Mol Fraction line

## Lever Rule

$$f^a = \frac{x_B}{x_B^a + x_B^b}$$

$$x_B^a = (x_B^a)(1-f^a)$$

## Proof

$$\textcircled{1} f_B + f_a = 1$$

$$\textcircled{2} x_B = f_a x_B^a + f_B x_B^b$$



Substitute & solve

## Gibbs Energy of Mixing

$$G = \sum_k \mu_k x_k + \sum \Delta H_k x_k$$

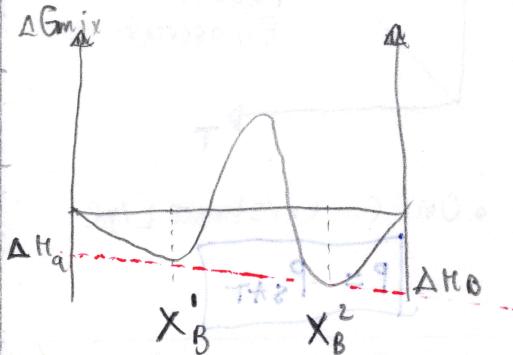
$$\Delta G = \sum \Delta H_k x_k$$

\* Graphic method to find  $\Delta H$ ,  $\Delta G$  from Gibbs Plot

\* Graphic method to find  $\Delta H$ ,  $\Delta G$  from  $\Delta G$  Plot

## 2 Phase Equilibrium

\* look for common tangent on Free Energy Diagram



## Ideal Solution Model

$$\Delta H_k = RT \ln(x_k)$$

↓ change in chemical potential  
↑ T, increase solubility  
Due to mixing

## Simple Regular Solution Model

$$\Delta H_k = RT \ln(x_k) + \text{[ ] } x_A x_B$$

## Reference States

- Solving 2 Phase (For co-existence in liquid phase)  $T_m, G_{cL}$
- (1)  $H_{Si}^d = H_{Si}^L$
- II

$$H_{Si}^0 + \Delta H_{Si}^{a \rightarrow L} + \Delta H_{Si}^{L}$$

(2)

$$H_{Ge}^d = H_{Ge}^0 + \Delta H_{Ge}^{a \rightarrow L}$$

## Simplifying Assumptions

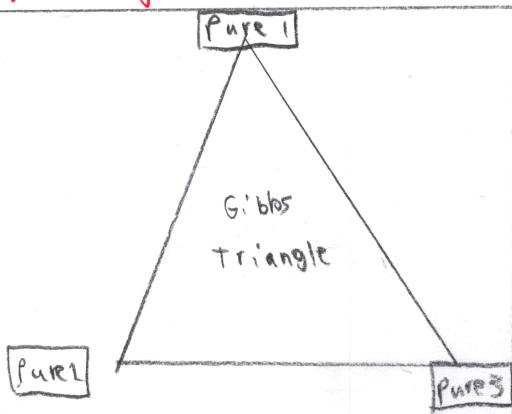
• AT transition  $\Delta G^{a \rightarrow L} = 0$

• if  $\Delta c_p = 0$  ( $\Delta H^{a \rightarrow L}$ ,  $\Delta S^{a \rightarrow L}$ ) are constant

$$\Delta G_k^{a \rightarrow L} (T) = \Delta S (T_0 - T)$$

↓  
transition temp

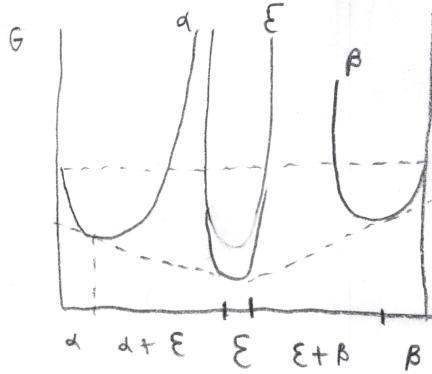
# Ternary Phase Diagram



$$D.o.F = 5 - P_h$$

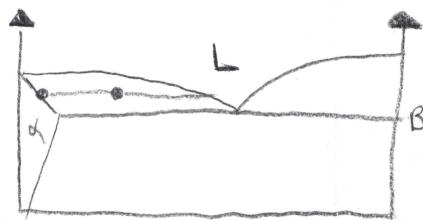
## Line Compounds

- An intermediate phase that forms at a specific range of temperatures at a fixed temperature



## Solutions vs. Reactions

### Solution Modeling



- At Equilibrium  $\Delta G = 0$

$$\begin{aligned} H_A^L &= H_A^0 \rightarrow H_A^0 + \Delta H_{A\text{ mix}}^0 \\ &= H_A^0 + \Delta H_A^{0,L} + \Delta H_{A\text{ mix}}^L \end{aligned}$$

## Gas Phase Reactions

$$\dot{n}_i = H_i^0 + RT \ln(P_i/P_{i0})$$

$$K_p = \frac{(P_c)^c}{(P_A)^a (P_B)^b} = e^{-\Delta G_0/RT}$$

## ThermoDynamics 3

### Oxidation & Ellingham Diagrams

- You Use Temperature & Oxygen concentration to control Equilibrium

### Modeling Assumptions:

- Metal Oxide we'll treat as pure components w/ no Pressure Dependence
- \* We model  $O_2$  as an ideal gas, chemical Potential depends on Partial Pressures

### Ellingham Diagram

- Simplifying Assumptions of

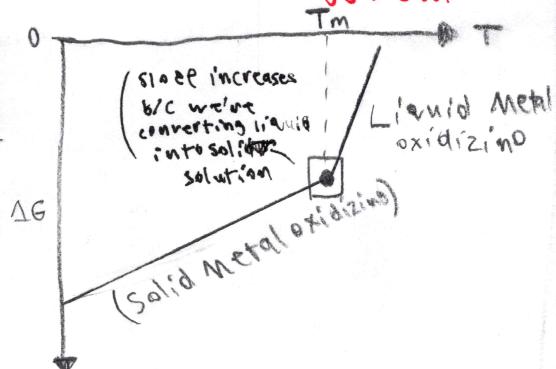
$$K_p = e^{(-\Delta G^\circ/RT)}$$

- $\Delta H^\circ(T)$  is constant

↳ Dominated by heat of oxide formation

- $\Delta S^\circ(T)$  is constant

↳ Dominated by Entropy of Removal of Gas from System



### Oxygen Pressure Scale

↳ if  $P_{O_2} > P_{O_2, E_a}$  (everything oxidizes)

↳ if  $P_{O_2} < P_{O_2, E_a}$  (Everything Reduces)

