BASIC BASIC BASIC

The fact/knowledge every PhD/materials science scientist should know is……

Prof. Soffa

Here what I will try to do is to classify and mentioned every basic **question** to diagnose the basis. As they are all basic questions, you can simply wiki/google for the answers. The aim is to classify all over the materials science field. This can be seen as a syllabus for the whole field and all kinds of quiz for different parts. Here I will focus on "double basics": basic concepts and basic skills which is due to my traditional Chinese education philosophy. Any contributed edition is very welcome.

Fundamental sides:

The big picture of four core courses:

Crystal→Defect: **fundamental** and **universal** knowledge about how materials "constitute" in perfect or defect.

Thermodynamics→Kinetics: **fundamental** and **universal** knowledge about how materials "exist" in equilibrium or process.

Application sides:

Processing/Structure/Properties/Performance:

structure materials and mechanical properties

functional materials (EMOp) and electrical, magnetic, optical, (thermal), properties

phase transformation and materials processing

special materials: ceramic, polymer, composites

special "reaction": fracture, corrosion(degradation)

Techniques to study MSE(see other slides):

Computational:

first-principle calculation: DFT

MD/MC simulation

CALPHAD

Machine learning

…

experimental:

Diffraction: x-ray(photon), neutron, electron

Microscopy: TEM SEM SPM

You have to integral the three parts, the fundamental and universal core knowledge (which means it's a little bit abstract), the application part(especially consider the industry potential application) and the detailed techniques to attack the problem.

Crystal/Electron(review HW as well, during the proposal?):

Crystal=lattice + basis

Crystal structure, 2D and 3D:

How many 2D crystal

What's the structure of $L1_0\,(L1_2)$? State it in lattice + basis. Example compounds? (Tetragonal P + basis AB)

What's the differences between HCP and FCC?

are related with different stacking

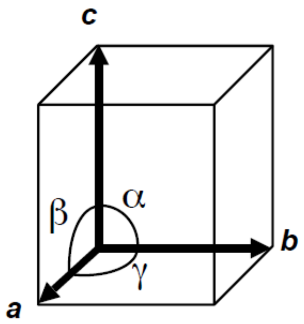
what's the structure for Diamond and ZincBlend?

Unit cell repeat and no overlaps

Primitive: smallest

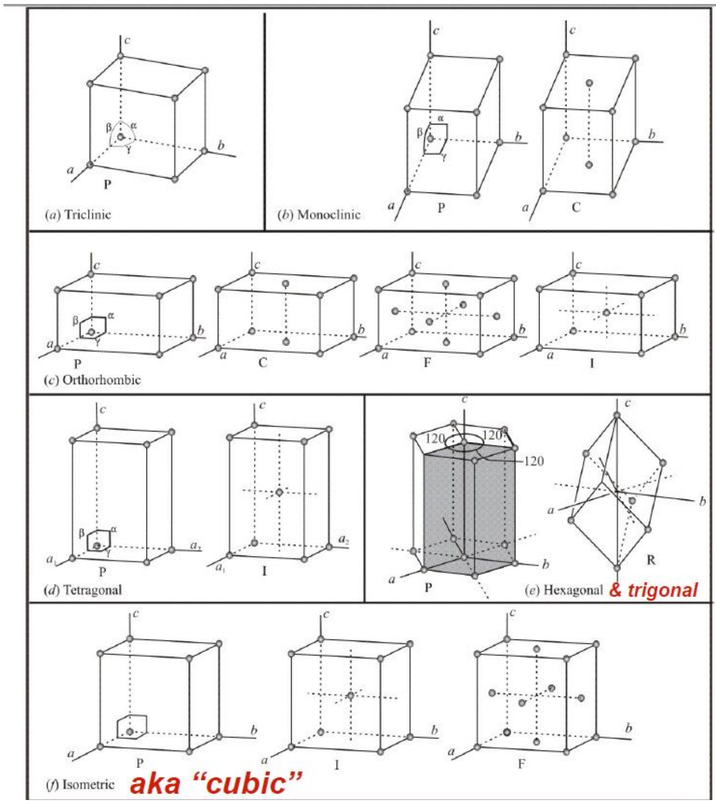
Conventional: better capture symmetry

Wigner-Seitz: primitive but in some specific method



Lengths of a, b, and c are the *lattice parameters*

System	*Lattice Parameters*	*Angles*	*Minimum Symmetry*
TRICLINIC	**a ≠ b ≠ c**	**$\alpha \neq \beta \neq \gamma \neq 90^\circ$**	**1 or $\bar{1}$**
MONOCLINIC	**a ≠ b ≠ c**	**$\alpha = \gamma = 90^\circ \neq \beta$**	**Single 2 or $\bar{2}$ (= m)**
ORTHORHOMBIC	**a ≠ b ≠ c**	**$\alpha = \beta = \gamma = 90^\circ$**	**Three 2's**
TETRAGONAL	**a = b ≠ c**	**$\alpha = \beta = \gamma = 90^\circ$**	**Single 4 or $\bar{4}$**
CUBIC	**a = b = c**	**$\alpha = \beta = \gamma = 90^\circ$**	**Four 3's or $\bar{3}$'s**
HEXAGONAL	**$a_1 = a_2 = a_3 \neq c$**	**$\alpha = \beta = 90^\circ$; $\gamma = 120^\circ$**	**Single 6 or $\bar{6}$**
TRIGONAL (RHOMB)	**a= b = c**	**$\alpha = \beta = \gamma \neq 90^\circ$**	**Single 3 or $\bar{3}$**



3D Bravais Lattices (14)

All the Bravais lattices can be built by stacking the 2D plane lattices.

The names here (e.g., "cubic I" instead of "BCC" are to distinguish lattices from crystal structures)

Explain:

i) **Why no cubic C?**
ii) **Why no tetragonal F?**

Hexagonal, Trigonal and Rhombohedral:

1. from the standpoint of symmetry, Hexagonal and Trigonal are cleanly distinguished: the min symmetry of trigonal is 3 while that of hexagonal is 6.

2. All trigonal crystals have a hexagonal lattice (next slide).

If the trigonal unit cell is primitive, then the lattice gets called ***Rhombohedral*** (!). Even so, since the hex cell is easier to visualize, it is often chosen as the conventional cell for display purposes.

Sometimes, the lattice is straight-up Hexagonal P, but the basis reduces the primary rotational symmetry from 6 to 3. This is still trigonal, but the UC is now $a=b\neq c$, $\alpha=\beta=90^\circ$, $\gamma=120^\circ$.

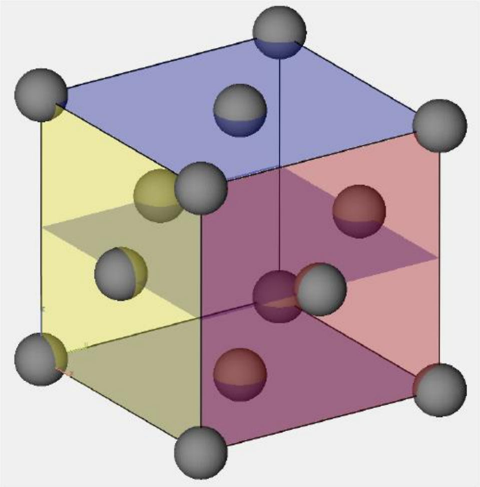
Miller Indices

To determine the Miller indices of any plane:

1. **It must not pass thru the origin**
2. **Find the intercept on each of the primary crystal axes, as a fraction of a, b and c**
3. **Take the reciprocal of these unitless intercepts**
4. **Get rid of fractions**
5. **Those are the Miller Indices (hkl)**

Families of Planes

Planes of the same *form* (=> atomic arrangements are identical) are denoted by {hkl}



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Crystallographic Directions

To determine the direction vector indices in any crystal:

1. **Determine the coordinates of the endpoint relative to the origin, or…**
2. **…use x_2-x_1, y_2 - y_1, z_2 - z_1 if the vector does not pass thru the origin**
3. **If you want the general direction, get rid of any fractions**
4. **Otherwise, if you care about specific lengths, include fractions as needed.**
5. **Those are the direction indices [uvw]**

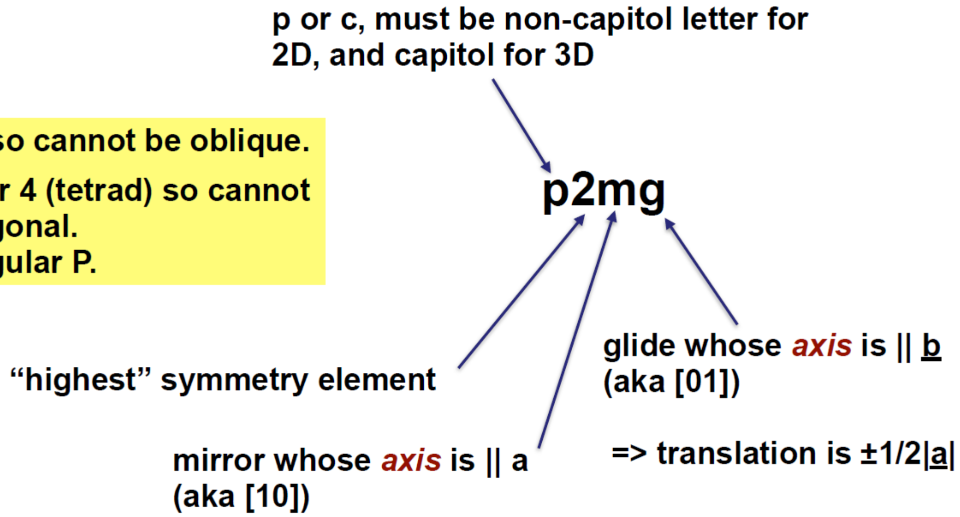
Symmetry

What’s the minimum symmetry for Cubic?

What’s in a name?

This has a mirror, so cannot be oblique.

It has no 3 (triad) or 4 (tetrad) so cannot be square or hexagonal.
=> must be rectangular P.



p or c, must be non-capitol letter for 2D, and capitol for 3D

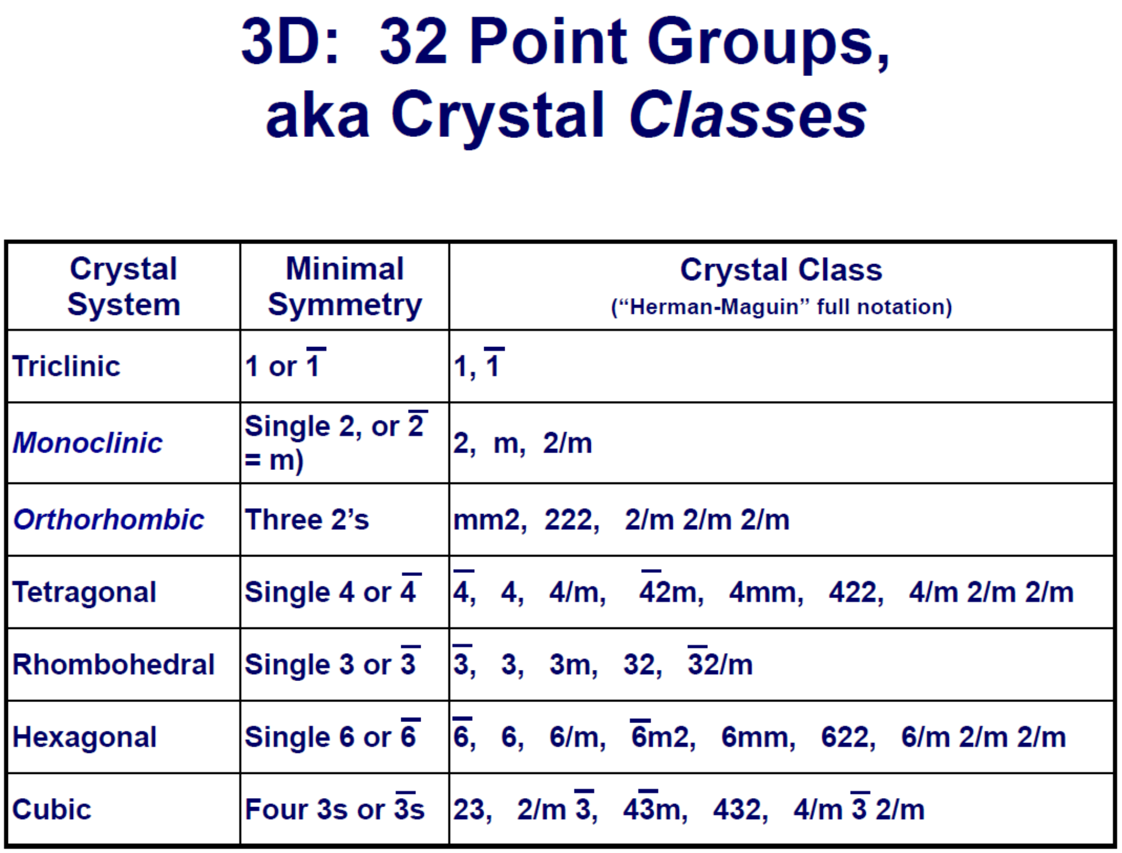
p2mg

“highest” symmetry element

mirror whose *axis* is || a (aka [10])

glide whose *axis* is || b (aka [01])

=> translation is ±1/2|a|



3D: 32 Point Groups, aka Crystal *Classes*

Crystal System	Minimal Symmetry	Crystal Class (“Herman-Maguin” full notation)
Triclinic	1 or $\bar{1}$	1, $\bar{1}$
Monoclinic	Single 2, or $\bar{2}$ = m)	2, m, 2/m
Orthorhombic	Three 2’s	mm2, 222, 2/m 2/m 2/m
Tetragonal	Single 4 or $\bar{4}$	$\bar{4}$, 4, 4/m, $\bar{4}2m$, 4mm, 422, 4/m 2/m 2/m
Rhombohedral	Single 3 or $\bar{3}$	$\bar{3}$, 3, 3m, 32, $\bar{3}2/m$
Hexagonal	Single 6 or $\bar{6}$	$\bar{6}$, 6, 6/m, $\bar{6}m2$, 6mm, 622, 6/m 2/m 2/m
Cubic	Four 3s or $\bar{3}$s	23, 2/m $\bar{3}$, $4\bar{3}m$, 432, 4/m $\bar{3}$ 2/m

Complex crystals

Naming crystal structures:

1. **Archetype**
2. **Strukturbericht**
3. **Space Group**

A: elements (A1 = FCC, A2 = BCC, A3 = HCP, A4 = DC .... A15)

B: 1:1 alloys/compounds (B1 = NaCl, B2 = CsCl, B3 = zinc blende, B4 = wurtzite ...)

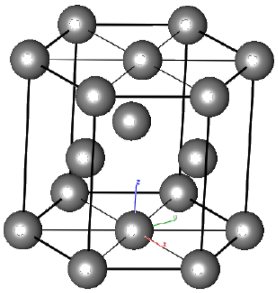
C: 2:1 alloys/compounds

D: other stoichiometry ($D0_n$, $D1_n$,...$D10_n$)

E: ternaries

L: ordered alloys (there are 6, incl. $L1_0$, $L1_2$)

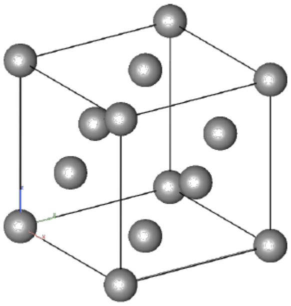
Close-Packed Structures are Special



Hexagonal Close-Packed (HCP)
$P6_3mmc$

2 atoms per *primitive* UC:
0,0,0
1/3, 2/3, 1/2

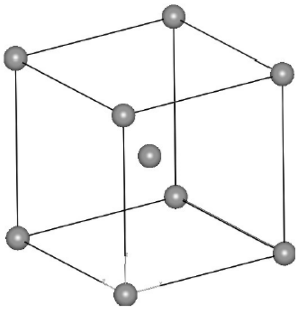
APF = 0.74
CN = 12 which are “a” apart



Face-Centered Cubic (FCC)
Fm$\underline{3}$m

4 atoms per *conv.* UC:
0,0,0
1/2, 1/2, 0...

APF = 0.74
CN = 12 which are (√2/2) apart
NNN = 6 that are 1.41*NN



Body-Centered Cubic (BCC)
Im$\underline{3}$m

2 atoms per *conv.* UC:
0,0,0
1/2, 1/2, 1/2

APF = 0.68
CN = 8 which are (√3/2) apart
NNN = 6 that are 1.15*NN

Note the difference of stacking in HCP and FCC

Interstitial and substitute. Tetrahedra and octahedral site

Diffraction

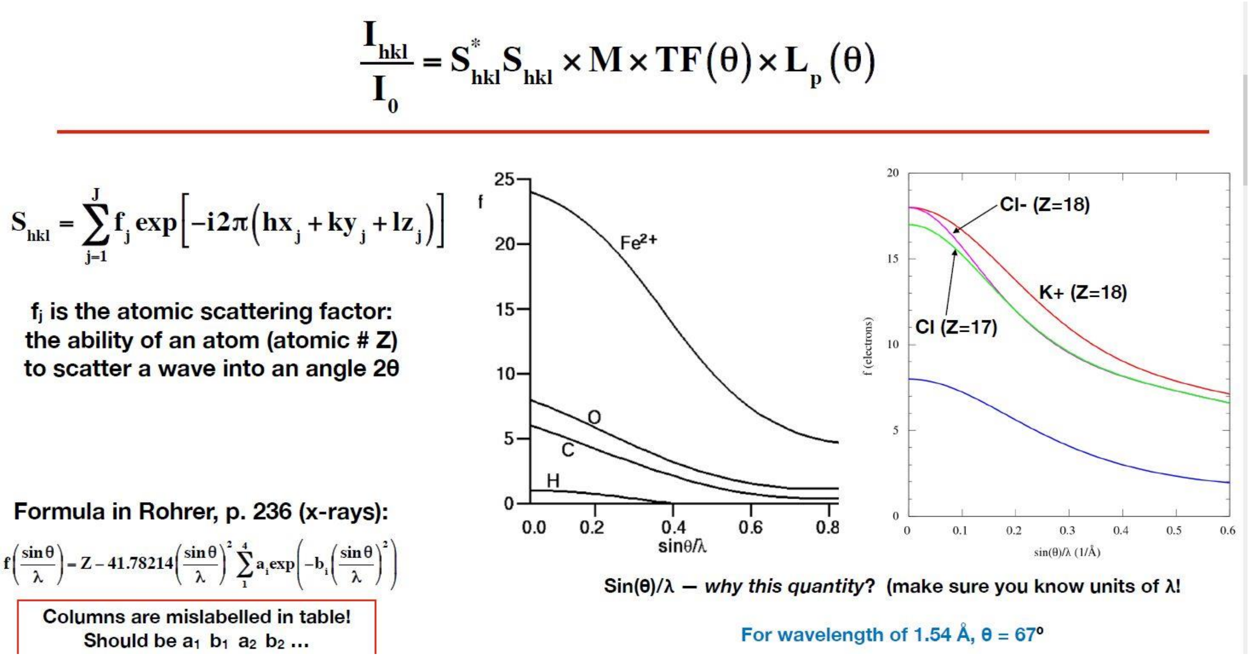
What’s the structure factor?

Why we can’t see (001) in bcc-fe electron diffraction pattern?

What’s the relation for the reciprocal space of bcc and fcc?

State the Bragg’s law clearly?

State the basic source for the diffraction? Electron/x-ray(photon)/ neutron



$$\frac{I_{hkl}}{I_0} = S^{*}_{hkl} S_{hkl} \times M \times TF(\theta) \times L_p(\theta)$$

$$S_{hkl} = \sum_{j=1}^{J} f_j \exp\left[-i2\pi\left(hx_j + ky_j + lz_j\right)\right]$$

f_j is the atomic scattering factor: the ability of an atom (atomic # Z) to scatter a wave into an angle 2θ

Formula in Rohrer, p. 236 (x-rays):

$$f\left(\frac{\sin\theta}{\lambda}\right) = Z - 41.78214\left(\frac{\sin\theta}{\lambda}\right)^2 \sum_{1}^{4} a_i \exp\left(-b_i\left(\frac{\sin\theta}{\lambda}\right)^2\right)$$

Columns are mislabelled in table! Should be a_1 b_1 a_2 b_2 …

Sin(θ)/λ — *why this quantity*? (make sure you know units of λ!

For wavelength of 1.54 Å, θ = 67°

The Reciprocal Lattice

The reciprocal lattice:

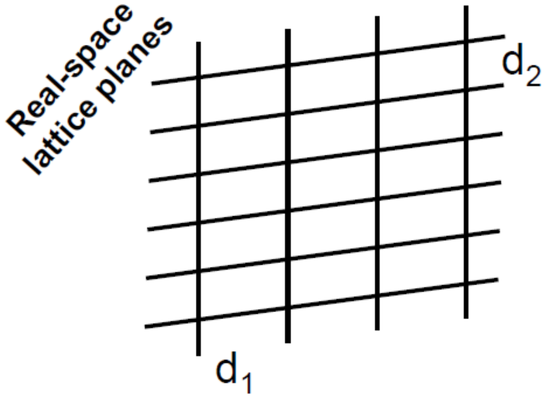
A complete geometric description of diffraction conditions

Represents all the sets of planes in a crystal —> explicit periodicity

Fourier transform of the real-space lattice into momentum space

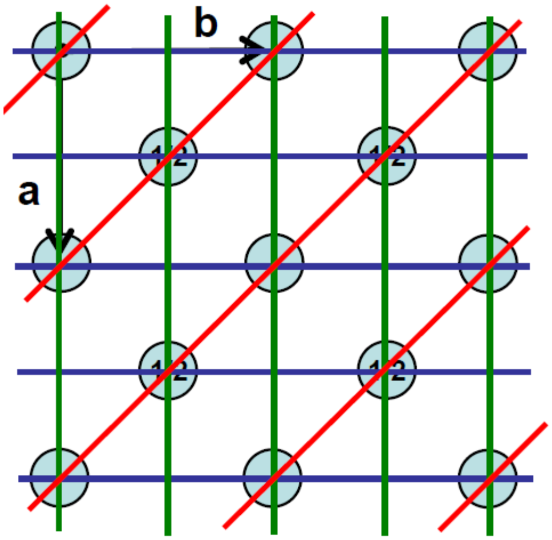
Important for electron bandstructure calculations

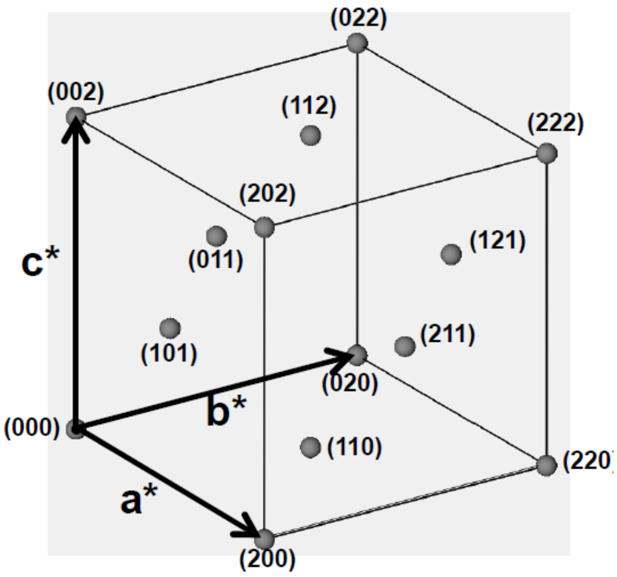
Constructing the reciprocal lattice:



1. Assign an origin to the real lattice.
2. Identify the fundamental plane spacings in or bounding the unit cell.
3. Draw a vector normal to each set, attached to the origin.
4. Make the length = $2\pi/d_{hkl}$.
5. Label RL points with hkl indices they arose from.

Example: **Cubic I lattice**





Reciprocal lattice of Cubic I is Cubic F!

$$\mathbf{d}^*_{hkl} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$$

Formal RL Definition

The mathematical definition of the unit cell vectors for the reciprocal lattice (**a***,**b***,**c***), in terms of the real space unit cell vectors (**a**, **b**, **c**):

$$a^* = \frac{b \times c}{a \bullet b \times c} 2\pi \qquad b^* = \frac{c \times a}{a \bullet b \times c} 2\pi \qquad c^* = \frac{a \times b}{a \bullet b \times c} 2\pi$$

BUT:

must use primitive lattice vectors

What is always true: **a* · a = 2π, a* · b = 0, a* · c = 0, etc.**

Key Points to Understand:

The reciprocal lattice points (and vectors, G_{hkl}) simply represent all sets of (hkl) planes in the real lattice

> **The spacing of the planes is inversely-related to the length of the reciprocal lattice vector G_{hkl}.**
>
> **Each G_{hkl} is normal to the (hkl) planes it represents.**

Apparent "missing indices" (e.g., (100) in BCC and FCC) are only the result of our choice of a conventional unit cell, and the resulting labels we apply to the planes.

There is a unique RL for each BL (but not for each crystal structure!)

=> 14 RL's, not 230….

Peak's position----lattice

Peak's intensity----basis

Many peak? polycrystal

Electronic structure (not too much)

What's the Brillouin zone?

What's the Fermi surface?

Understand some basic / essential quantum concepts for electron energy levels in solids.

=> where do energy bands come from?
=> how do you fill energy bands with electrons?
=> where do band gaps come from, and what are their implications?
=> what is the Fermi energy/Fermi surface?
=> what are Brillouin Zones?

How I will develop this:

1. Classical electrons - "the free electron gas"

   Pass: Electrical conductivity
   Fail: Heat capacity, mean free path

2. Quantum free electrons - "electrons in a box"

   Pass: Electrical conductivity, heat capacity
   Fail: No insulators

3. Quantum near free electrons - a weak potential to represent the darn atoms

   Pass: Insulators vs. metals
   Fail: Still highly approximate

Defects:

Basic elastic mechanics:

What’s Young’s modulus? And Stress-strain behavior?

Point defect:

What’s the form of point defects?

Frenkel and Schottky

defect-free crystals do not exist due to equilibrium vacancy equilibrium

Doping in semiconductor…

Discuss about the Brouwer diagram?

Dislocation:

What’s the dislocation? What’s the Burgers vector? What’s the slip plane?

What’s the difference between edge and screw dislocations?

What's the Peach-Kohler force?

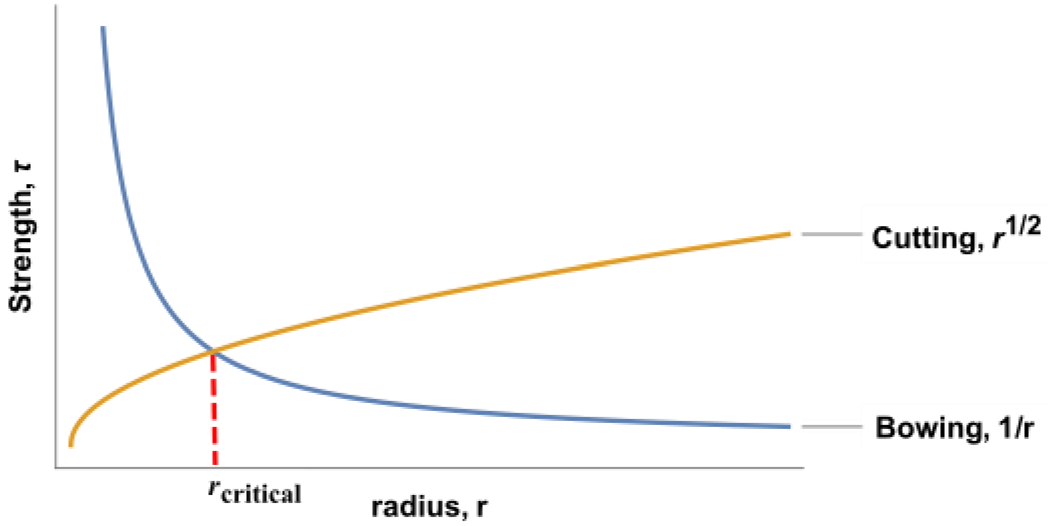
What's the partial dislocation?

What's the stacking fault?

What's the Orowan mechanism?

What's the friedel spacing?

What's the precipitation hardening? State your understanding about the figure below.



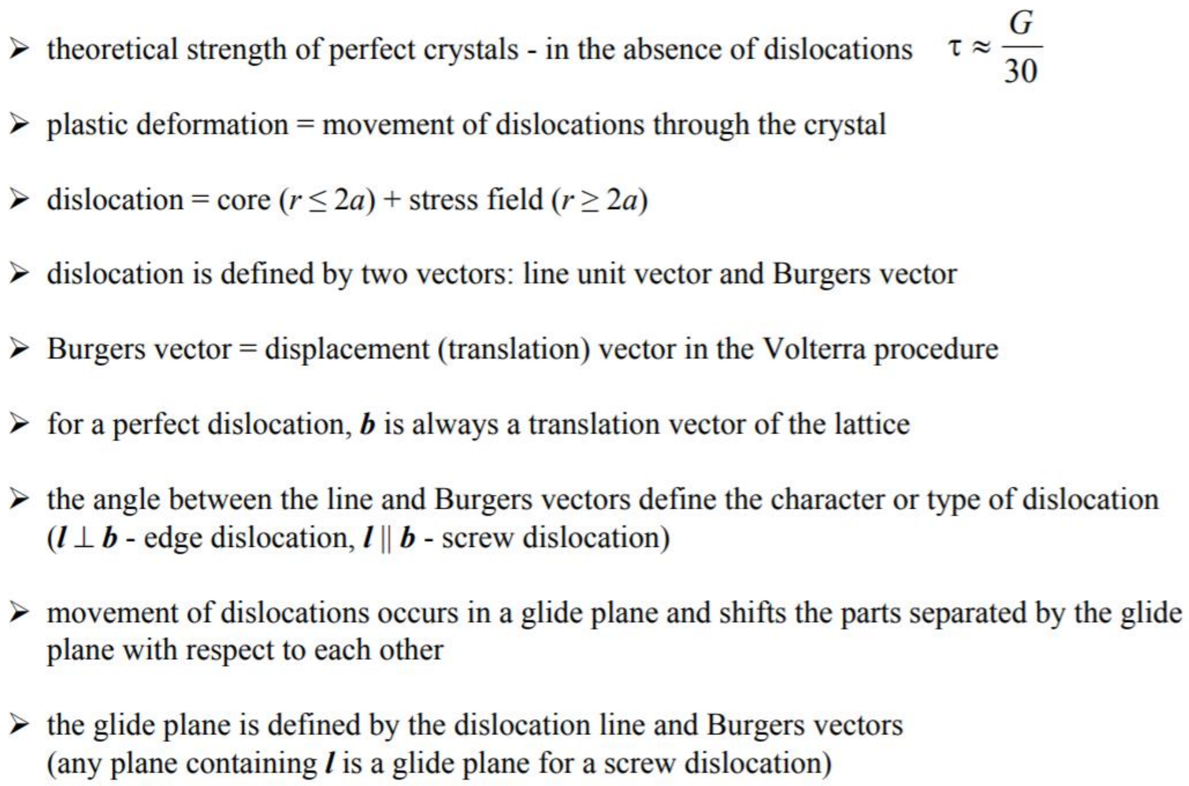
Talk about the dislocation core structure, the Peierls-Nabarro model?

What's the cross-slip of dislocation?

What's the line tension?

Self-force

Illustrate the different types of mechanisms for the movement of dislocation?



- theoretical strength of perfect crystals - in the absence of dislocations $\tau \approx \frac{G}{30}$
- plastic deformation = movement of dislocations through the crystal
- dislocation = core ($r \leq 2a$) + stress field ($r \geq 2a$)
- dislocation is defined by two vectors: line unit vector and Burgers vector
- Burgers vector = displacement (translation) vector in the Volterra procedure
- for a perfect dislocation, ***b*** is always a translation vector of the lattice
- the angle between the line and Burgers vectors define the character or type of dislocation ($\boldsymbol{l} \perp \boldsymbol{b}$ - edge dislocation, $\boldsymbol{l} \parallel \boldsymbol{b}$ - screw dislocation)
- movement of dislocations occurs in a glide plane and shifts the parts separated by the glide plane with respect to each other
- the glide plane is defined by the dislocation line and Burgers vectors (any plane containing ***l*** is a glide plane for a screw dislocation)

“image” torque???

Line tension

What’s the estimated stress field of dislocation? What’s the estimated energy of dislocation? Which means the feature of dislocation from energy and stress field

$$\boldsymbol{\sigma \sim \frac{b}{r}}$$

$$\boldsymbol{E_s = \frac{\mu b^2}{2}}$$

$$\boldsymbol{E_e = \frac{\mu b^2}{[2(1-v)]}}$$

μ shear modulus, v Poisson ratio

$$\boldsymbol{f_{climb} = \sigma b}$$

$$\boldsymbol{f_{glide} = \tau b}$$

$$\boldsymbol{f} = \boldsymbol{b\sigma\xi}$$

What's the Frank's rule?

typical movement of dislocation?

Climb and glide?

Climb is achieved by point defect at high temperature

Cross-slip of screw dislocation: overcome an activation barrier

Rare event

interaction between dislocation?

Based on Peach-koehler force

Attraction or Repulsive

Peach - Koehler

Peach-Koehler forces, interaction between dislocations lead to strengthening:

Pile up

Taylow hardening equation

Orowan relation

Orowan equation

Partial dislocation:

Why perfect to partial dislocation？

Perfect to partial separated by stacking faults to reduce energy

What’s antiphase boundary?

Dislocation core?

What’s the basic idea about Peierls-Babarro model?

Supplement the center region with the function, without the sigma comes to infinite

disregistry

in order to using this for partial dislocation energy

generalize the it with disreqistry with the generalized stacking fault energy

$$\sigma_{xy}(x, y = 0) = \frac{\mu b}{2\pi(1 - v)} \frac{x}{x^2 + \xi^2}$$

No stable stacking faults in BCC structure???

The elastic field of Solute and dislocation interaction?

Cottrell atmosphere

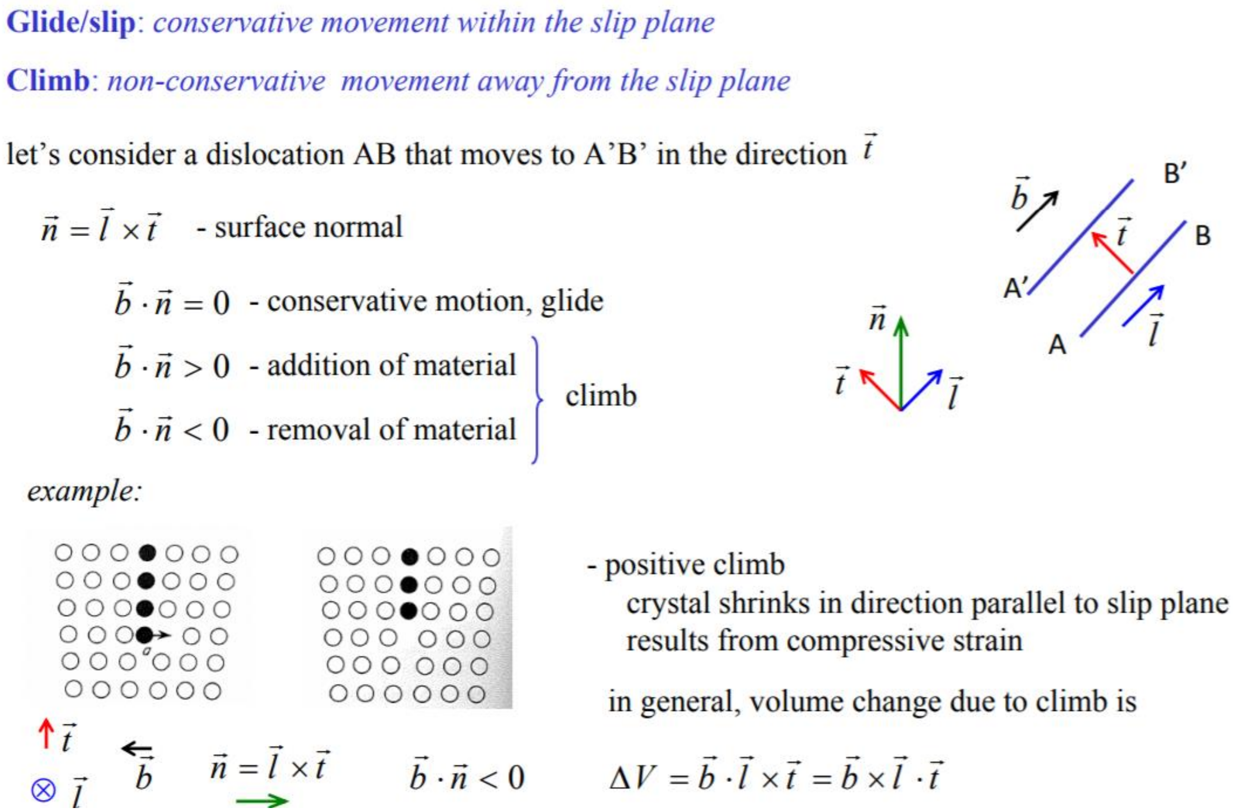
Pinning effect

Distinguish Glissile and prismatic dislocation loops?

at high T and/or presence of vacancy sinks the

prismatic loops of vacancy type will shrink

at vacancy supersaturation (c > c0) the loops can grows



Glide/slip: *conservative movement within the slip plane*

Climb: *non-conservative movement away from the slip plane*

let's consider a dislocation AB that moves to A'B' in the direction $\vec{t}$

$\vec{n} = \vec{l} \times \vec{t}$ - surface normal

$$\vec{b} \cdot \vec{n} = 0 \text{ - conservative motion, glide}$$

$$\left.\begin{array}{l} \vec{b} \cdot \vec{n} > 0 \text{ - addition of material} \\ \vec{b} \cdot \vec{n} < 0 \text{ - removal of material} \end{array}\right\} \text{climb}$$

example:

- positive climb
  crystal shrinks in direction parallel to slip plane
  results from compressive strain

in general, volume change due to climb is

$$\Delta V = \vec{b} \cdot \vec{l} \times \vec{t} = \vec{b} \times \vec{l} \cdot \vec{t}$$

(1) slip: *conservative movement* of dislocations perpendicular to $\boldsymbol{b} \times \boldsymbol{l}$, i.e., *within the slip plane*

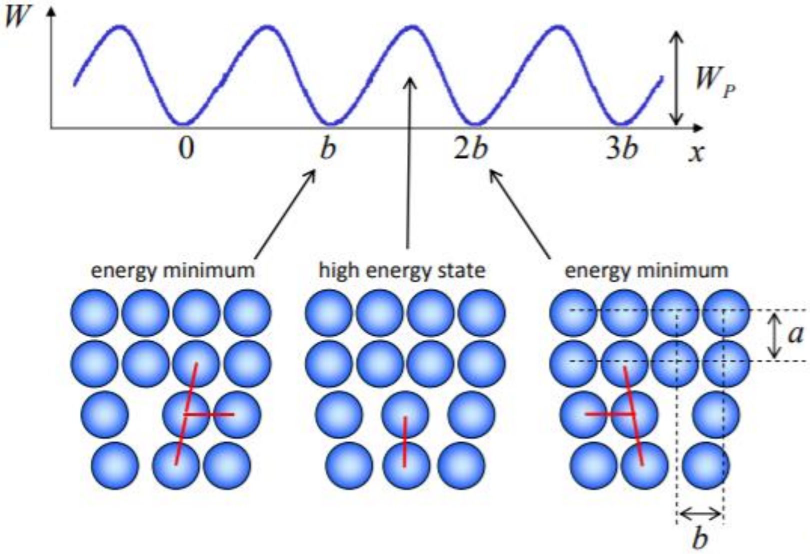
- the motion is reversible - if the sign of τ is reversed, the dislocation can move in the opposite direction and eventually restore the original configuration
- movement does not involve point defects
- an edge or mixed dislocation has only one slip plane defined by $\boldsymbol{b}$ and $\boldsymbol{l}$
- for screw dislocation, the number of slip planes is defined by its orientation and structure of the crystal (typically 2-4 easy slip planes)
- motion of a screw dislocation is always conservative

(2) climb: *non-conservative movement* of dislocations *away from the slip plane*

- the motion cannot be easily reversed - simple change of sign of τ does not reverse the process since additional work has to be done to create point defects
- movement is only possible with the help of point defects (vacancies or interstitials)
- climb is slow (involves diffusion of point defects) and has a strong dependence on T
- direct contribution of climb to the deformation rate $\dot{\varepsilon} = b\rho v_{\mathrm{climb}}$ is typically small (except for mostly screw dislocation with small edge segments - jogs)
- climb plays an important role in plastic deformation since it enable dislocations circumvent otherwise insurmountable obstacles

Lattice resistance to glide: Peierls stress

periodicity of lattice translates into the periodic variation of energy as a function of displacement of the dislocation core along a direction of high symmetry - ***Peierls-Nabarro potential***



approximate evaluation:

$$W_P = \frac{Gb^2}{\pi K}\exp\left(-\frac{2\pi a}{Kb}\right)$$

$$W = W_0 - \frac{W_P}{2}\cos\left(\frac{2\pi x}{b}\right)$$

$$\tau_P = \frac{F_{\max}}{b} = -\frac{1}{b}\frac{dW}{dx}\bigg|_{\max} = \frac{\pi W_P}{b^2}$$

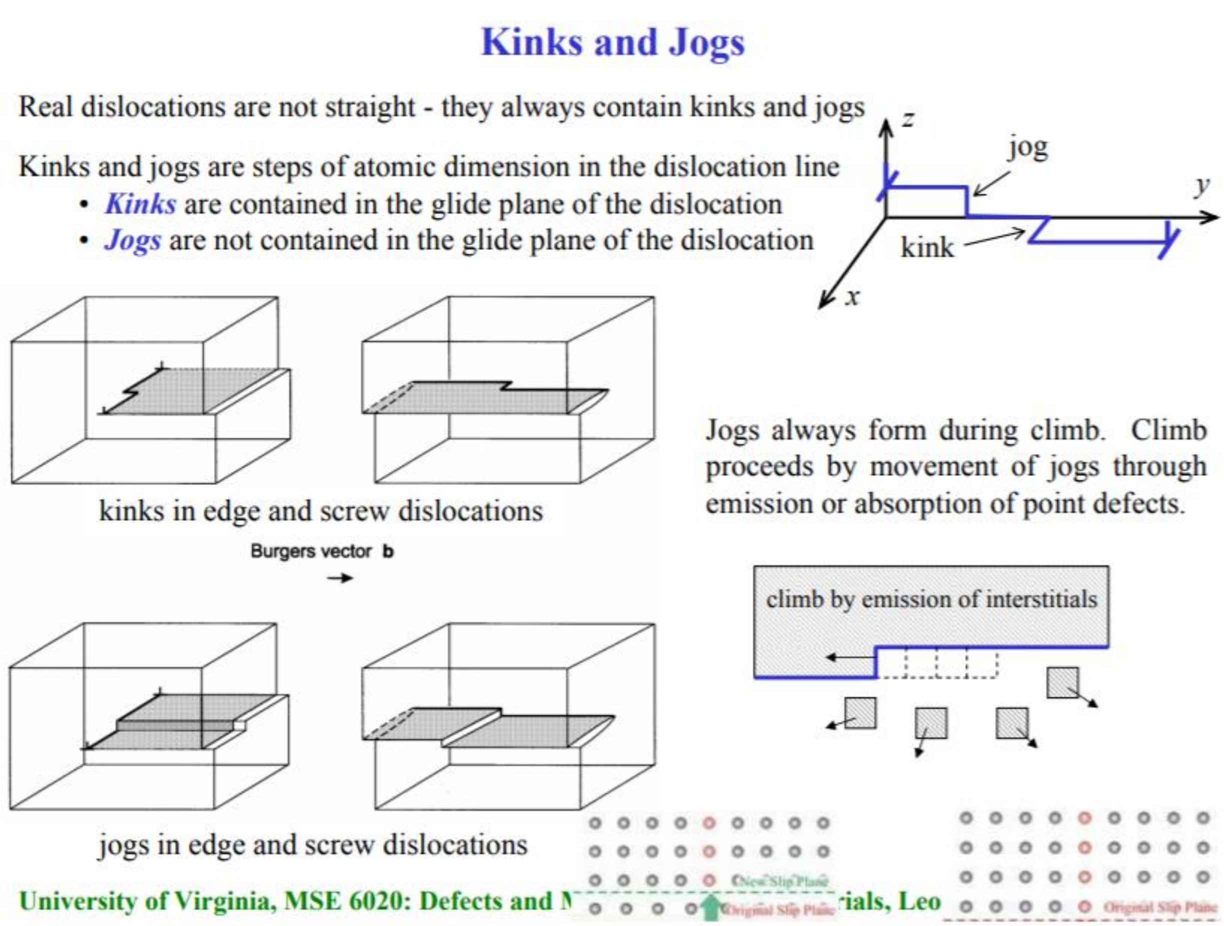
$$\tau_P = \frac{G}{K}\exp\left(-\frac{2\pi a}{Kb}\right)$$

$K = 1$ for screw dislocation
$K = 1 - \nu$ for edge dislocations

(W and W_P are per unit length)

- assuming a = b, $\nu = 1/3$, K = 2/3 (edge): $\tau_P \approx 1.2 \times 10^{-4}$ G $<< \tau_0 \approx$ G/6 … G/30
- slip tend to occur in most widely spaced planes (large *a*) and for small *b*

What’s the kinks and jogs?



Kinks and Jogs

Real dislocations are not straight - they always contain kinks and jogs

Kinks and jogs are steps of atomic dimension in the dislocation line

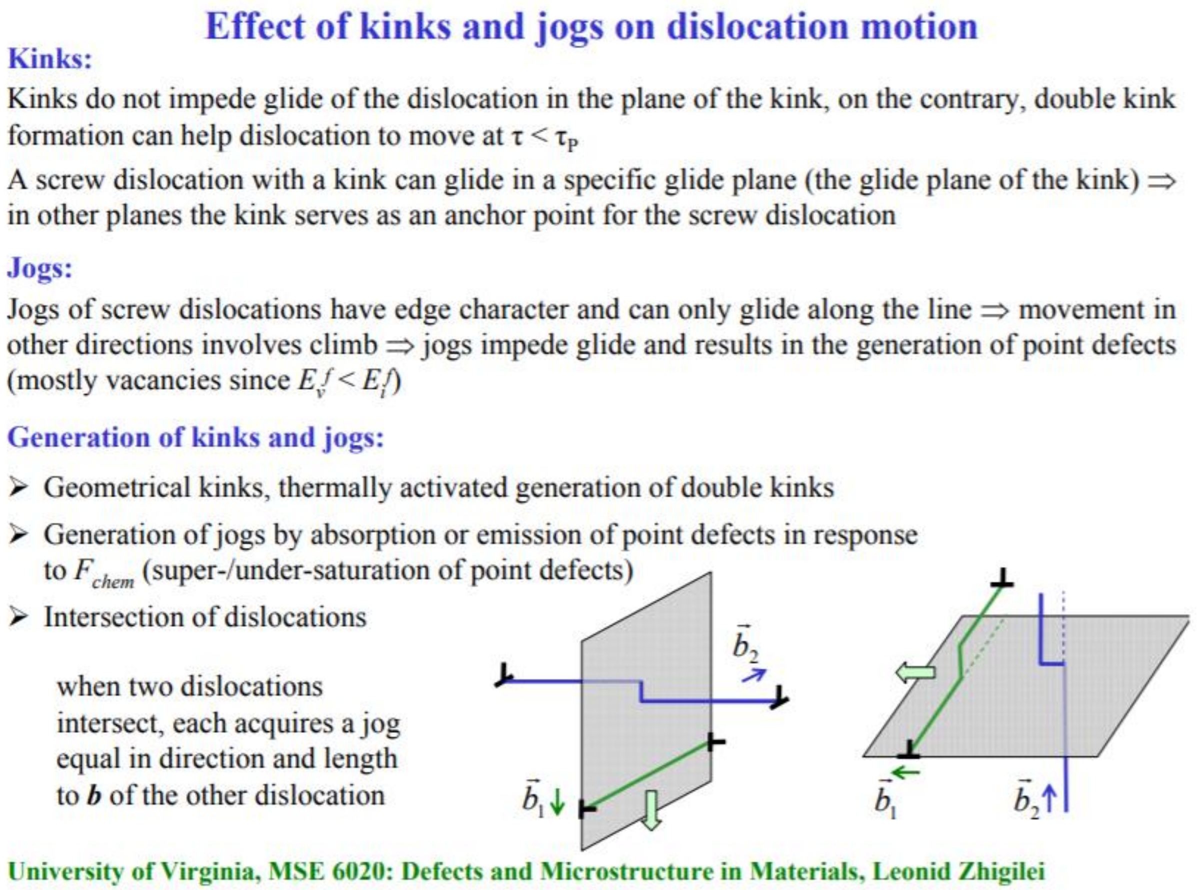
- ***Kinks*** are contained in the glide plane of the dislocation
- ***Jogs*** are not contained in the glide plane of the dislocation

kinks in edge and screw dislocations

jogs in edge and screw dislocations

Jogs always form during climb. Climb proceeds by movement of jogs through emission or absorption of point defects.

University of Virginia, MSE 6020: Defects and M **rials, Leo**



Effect of kinks and jogs on dislocation motion

Kinks:

Kinks do not impede glide of the dislocation in the plane of the kink, on the contrary, double kink formation can help dislocation to move at $\tau < \tau_P$

A screw dislocation with a kink can glide in a specific glide plane (the glide plane of the kink) ⇒ in other planes the kink serves as an anchor point for the screw dislocation

Jogs:

Jogs of screw dislocations have edge character and can only glide along the line ⇒ movement in other directions involves climb ⇒ jogs impede glide and results in the generation of point defects (mostly vacancies since $E_v^f < E_i^f$)

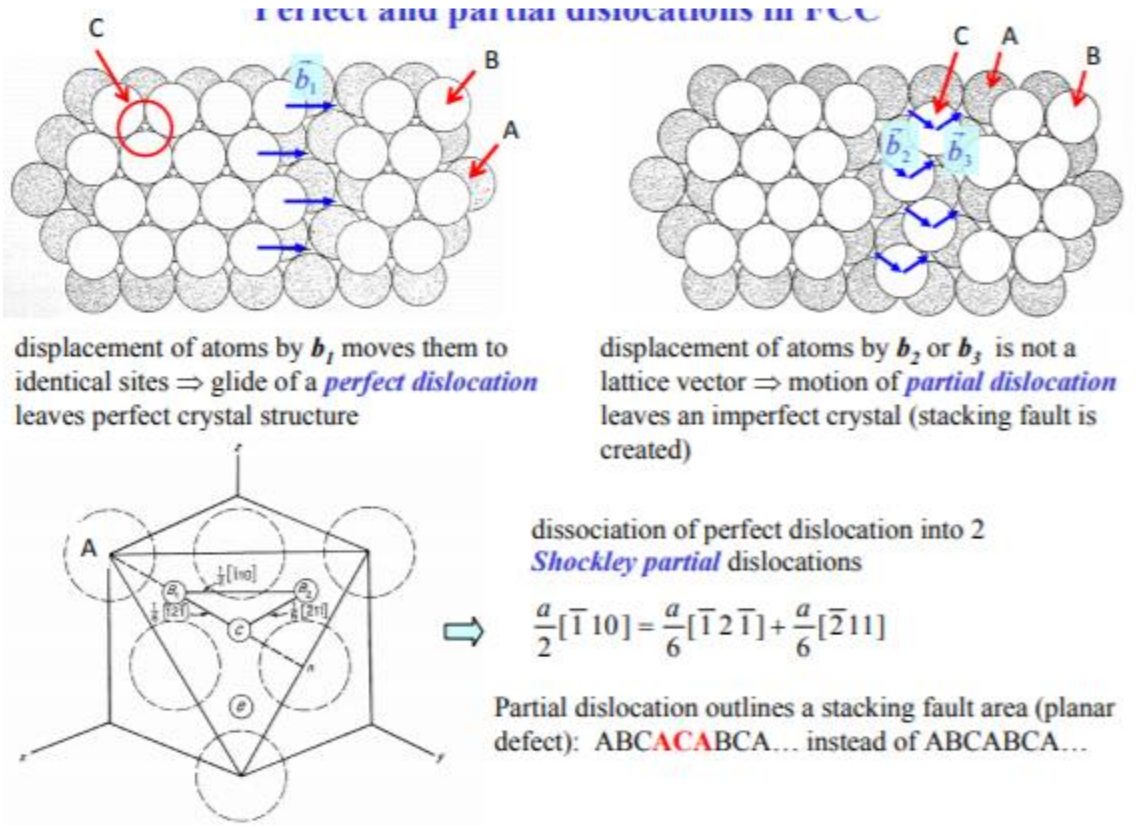
Generation of kinks and jogs:

- Geometrical kinks, thermally activated generation of double kinks
- Generation of jogs by absorption or emission of point defects in response to F_{chem} (super-/under-saturation of point defects)
- Intersection of dislocations

when two dislocations intersect, each acquires a jog equal in direction and length to ***b*** of the other dislocation

University of Virginia, MSE 6020: Defects and Microstructure in Materials, Leonid Zhigilei

Mechanisms of dislocation multiplication include: Frank-Read source, multiple crossslip, emission of dislocation from grain boundaries, etc.



Perfect and partial dislocations in FCC

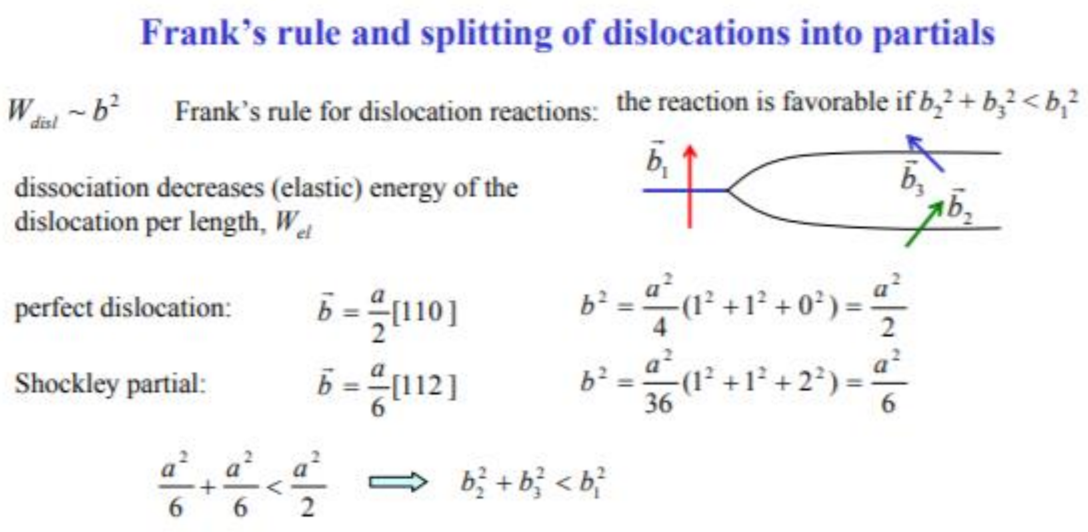
displacement of atoms by $\boldsymbol{b_1}$ moves them to identical sites ⇒ glide of a ***perfect dislocation*** leaves perfect crystal structure

displacement of atoms by $\boldsymbol{b_2}$ or $\boldsymbol{b_3}$ is not a lattice vector ⇒ motion of ***partial dislocation*** leaves an imperfect crystal (stacking fault is created)

dissociation of perfect dislocation into 2 ***Shockley partial*** dislocations

$$\Rightarrow \quad \frac{a}{2}[\bar{1}\,10] = \frac{a}{6}[\bar{1}\,2\,\bar{1}] + \frac{a}{6}[\bar{2}\,11]$$

Partial dislocation outlines a stacking fault area (planar defect): ABCACABCA… instead of ABCABCA…



Frank's rule and splitting of dislocations into partials

$W_{disl} \sim b^2$ Frank's rule for dislocation reactions: the reaction is favorable if $b_2^2 + b_3^2 < b_1^2$

dissociation decreases (elastic) energy of the dislocation per length, W_{el}

perfect dislocation: $\vec{b} = \frac{a}{2}[110]$ $\quad b^2 = \frac{a^2}{4}(1^2+1^2+0^2) = \frac{a^2}{2}$

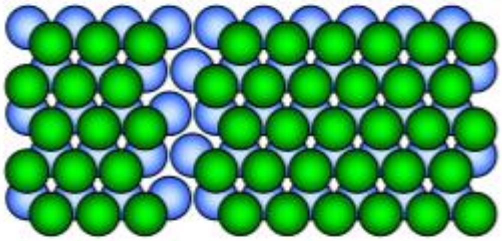
Shockley partial: $\vec{b} = \frac{a}{6}[112]$ $\quad b^2 = \frac{a^2}{36}(1^2+1^2+2^2) = \frac{a^2}{6}$

$$\frac{a^2}{6} + \frac{a^2}{6} < \frac{a^2}{2} \quad \Rightarrow \quad b_2^2 + b_3^2 < b_1^2$$

What's the Thompson tetrahedron?

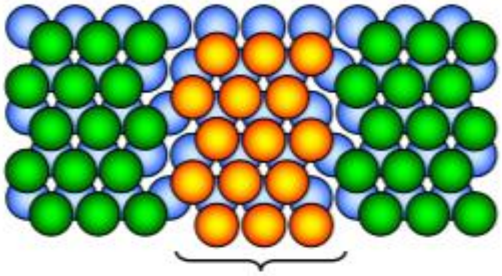
Stacking faults

perfect a/2[110] dislocation



two Shockley partials

$$\frac{a}{6}[211]+\frac{a}{6}[12\,\bar{1}]$$



Frank partial dislocation; Intrinsic vs. extrinsic stacking fault

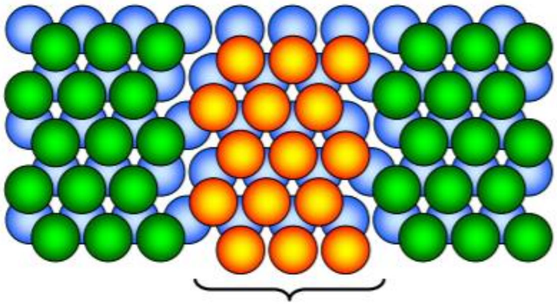
- *Frank partial dislocation* outlines a stacking fault formed by inserting or removing a region of close packed {111} plane.
- Frank partial has Burgers vector ***b*** = a/3<111> normal to the {111} plane.
- ***b*** = a/3<111> is not contained in one of the {111} glide planes ⇒ this is a *sessile* dislocation - cannot glide, can only climb
- Depending on whether the material is removed or added, the stacking fault outlined is called *intrinsic* or *extrinsic*

Frank partial dislocation; Intrinsic vs. extrinsic stacking fault

Intrinsic SF: can be generated by both Shockley or Frank partial dislocations

two Shockley partials

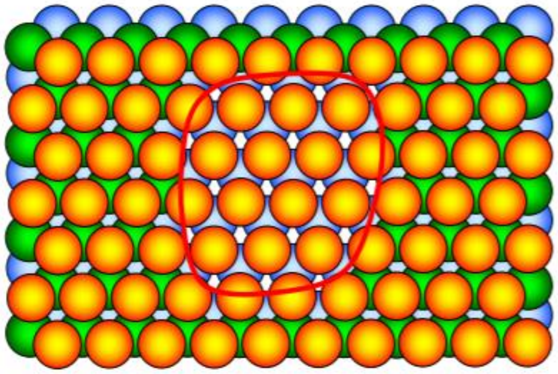
$$\vec{b} = \frac{a}{2}[110] = \frac{a}{6}[211] + \frac{a}{6}[12\bar{1}]$$



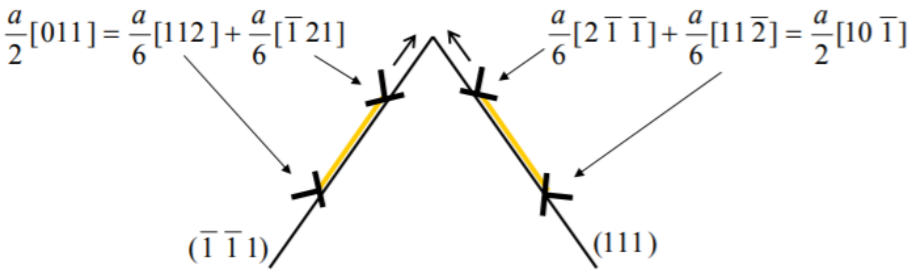
loop of negative Frank partial dislocation

(can be produced by collapse of platelet of vacancies)

$$\vec{b} = \frac{a}{3}[\bar{1}11]$$



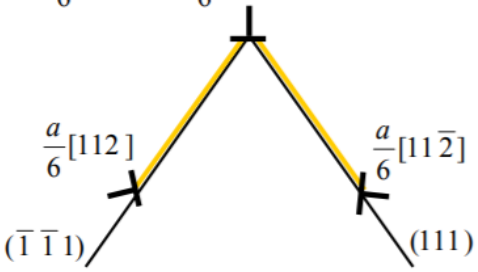
Examples of dislocation reactions: Lomer-Cottrell lock



$$\frac{a}{2}[011] = \frac{a}{6}[112] + \frac{a}{6}[\bar{1}21]$$

$$\frac{a}{6}[2\bar{1}\bar{1}] + \frac{a}{6}[11\bar{2}] = \frac{a}{2}[10\bar{1}]$$

$$\frac{a}{6}[\bar{1}21] + \frac{a}{6}[2\bar{1}\bar{1}] = \frac{a}{6}[110]$$



$$b^2 : \frac{a^2}{6} + \frac{a^2}{6} > \frac{a^2}{18}$$

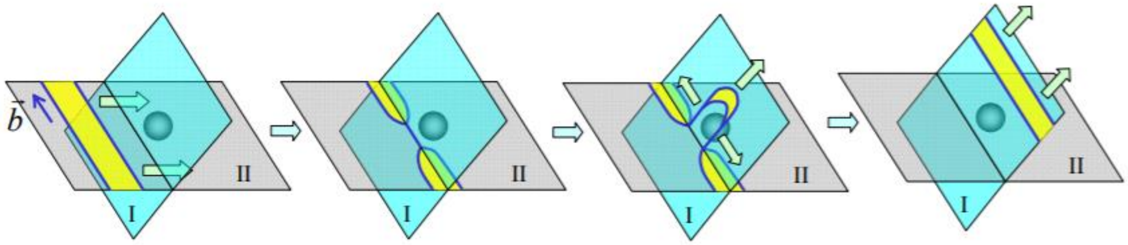
$\vec{b} = \frac{a}{6}[110]$ is perpendicular to the dislocation line $\vec{l} = [1\bar{1}0]$

(001) that contains both ***b*** and ***l*** is not a slip plane

the dislocation is sessile (*stair-rod* dislocation)

this sessile dislocation is called *Lomer-Cottrell lock* - it locks slip in the two slip planes

while a perfect screw dislocation in fcc (***b*** = a/2<110>) can glide in two {111} planes, a Shockley partial dislocation with ***b*** = a/6<112> lies in only one {111} plane ⇒ an extended dislocation cannot cross-slip without recombining into a perfect screw dislocation (formation of a *constriction*)



formation of a constriction requires energy and is easier for materials with large γ (small *d*)

cross-slip is one of the mechanisms of dislocation multiplication and propagation ⇒ more difficult cross-slip in materials with low γ leads to the build up of high internal stresses ⇒ may lead to more brittle behavior

Interface/2D defects

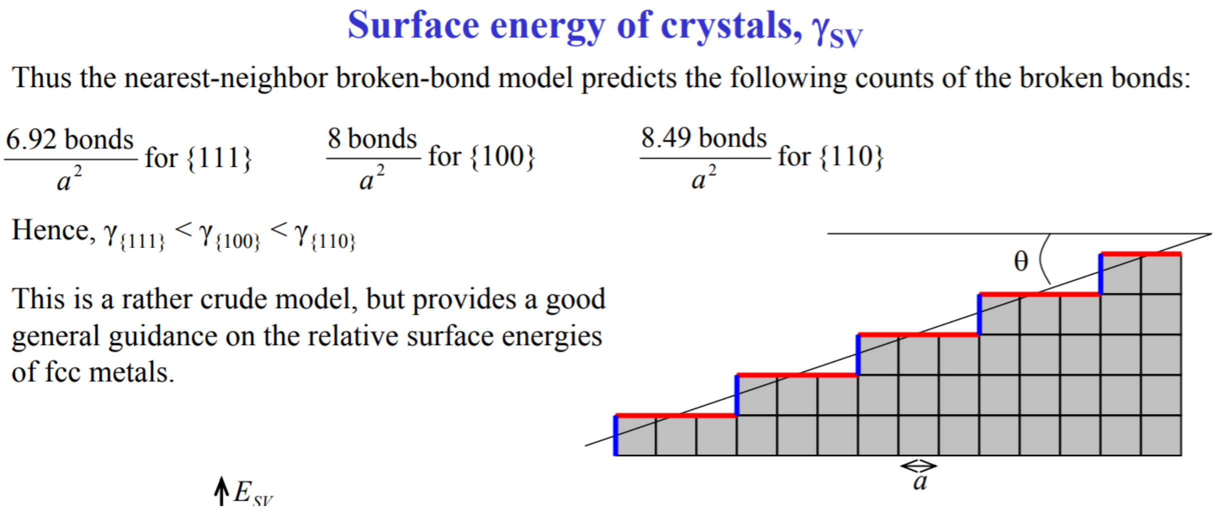
What’s the grain boundary? Distinguish low-angle grain boundaries and high-angle grain boundaries

Low: not block dislocation effectively, can be seen as edge dislocation array

High: block movement of dislocation

What’s the interface energy?

How different orientation affects interface energy?



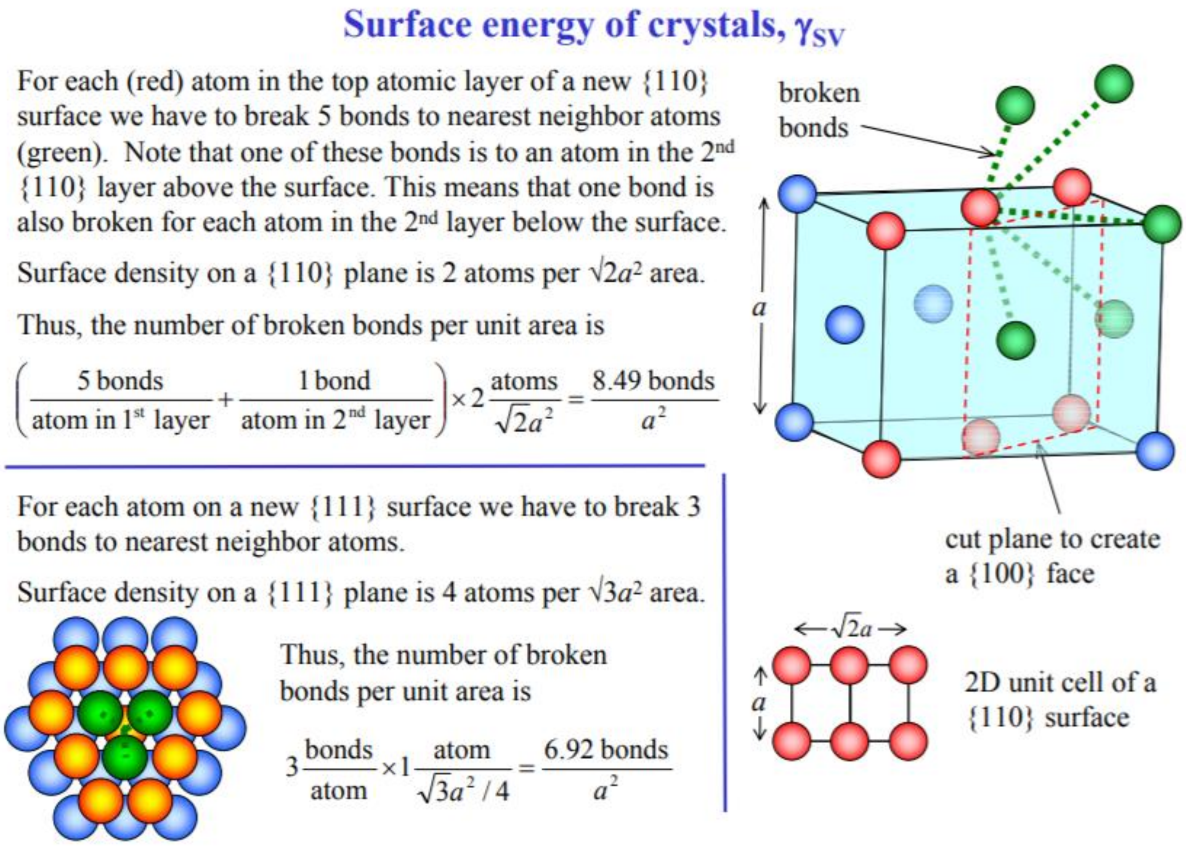
Surface energy of crystals, γ_{SV}

Thus the nearest-neighbor broken-bond model predicts the following counts of the broken bonds:

$$\frac{6.92 \text{ bonds}}{a^2} \text{ for } \{111\} \qquad \frac{8 \text{ bonds}}{a^2} \text{ for } \{100\} \qquad \frac{8.49 \text{ bonds}}{a^2} \text{ for } \{110\}$$

Hence, $\gamma_{\{111\}} < \gamma_{\{100\}} < \gamma_{\{110\}}$

This is a rather crude model, but provides a good general guidance on the relative surface energies of fcc metals.



Surface energy of crystals, γ_{SV}

For each (red) atom in the top atomic layer of a new {110} surface we have to break 5 bonds to nearest neighbor atoms (green). Note that one of these bonds is to an atom in the 2nd {110} layer above the surface. This means that one bond is also broken for each atom in the 2nd layer below the surface.

Surface density on a {110} plane is 2 atoms per $\sqrt{2}a^2$ area.

Thus, the number of broken bonds per unit area is

$$\left(\frac{5 \text{ bonds}}{\text{atom in } 1^{st} \text{ layer}} + \frac{1 \text{ bond}}{\text{atom in } 2^{nd} \text{ layer}}\right) \times 2\frac{\text{atoms}}{\sqrt{2}a^2} = \frac{8.49 \text{ bonds}}{a^2}$$

For each atom on a new {111} surface we have to break 3 bonds to nearest neighbor atoms.

Surface density on a {111} plane is 4 atoms per $\sqrt{3}a^2$ area.

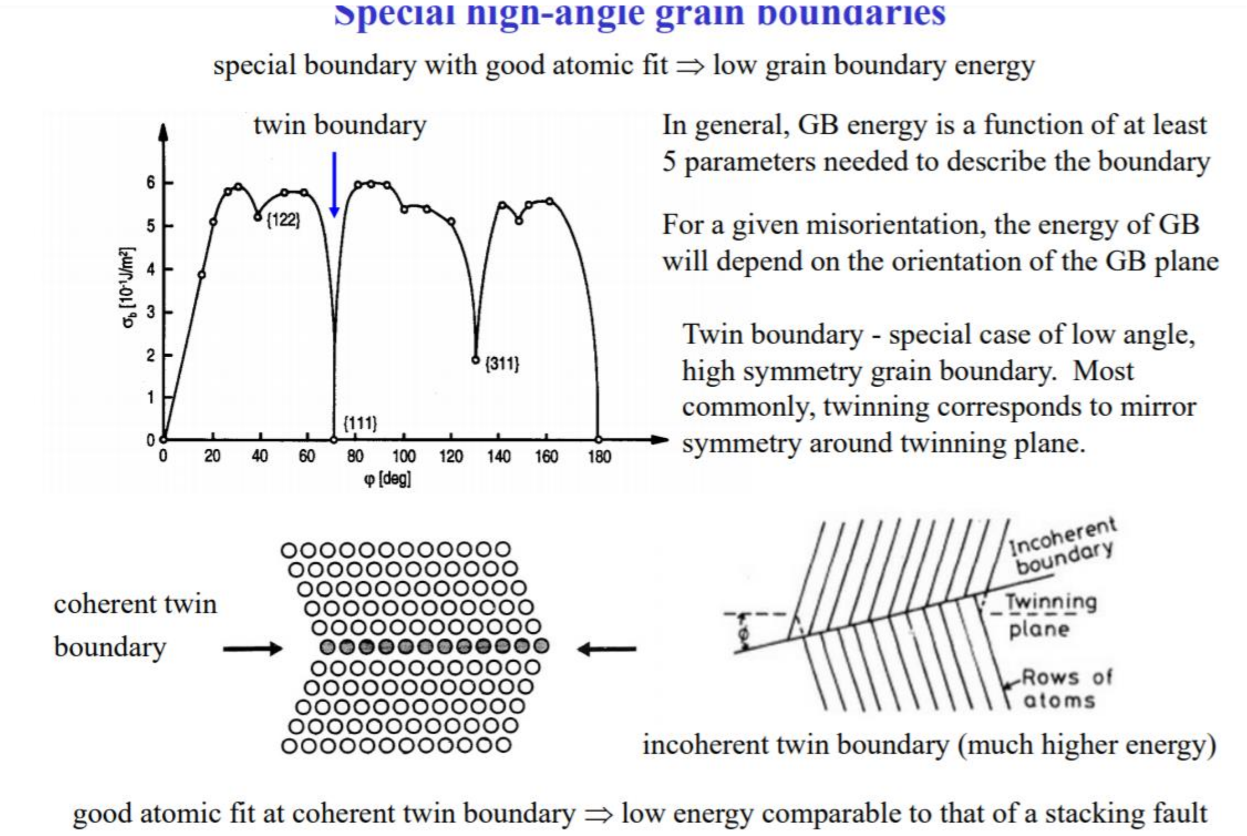
Thus, the number of broken bonds per unit area is

$$3\frac{\text{bonds}}{\text{atom}} \times 1\frac{\text{atom}}{\sqrt{3}a^2/4} = \frac{6.92 \text{ bonds}}{a^2}$$

What's the antiphase boundary? How is it related to stacking fault?

The surface energy of grain boundary???

for small θ, the distance between dislocations is large and the energy of the grain boundary, γGB, is proportional to the dislocation density as θ increases, the strain fields of dislocations increasingly cancel out and γGB tend to saturate σxx when θ approaches ~15º, core regions of the dislocations start to overlap and the description of GB in terms of dislocation wall is no longer useful



Special high-angle grain boundaries

special boundary with good atomic fit ⇒ low grain boundary energy

In general, GB energy is a function of at least 5 parameters needed to describe the boundary

For a given misorientation, the energy of GB will depend on the orientation of the GB plane

Twin boundary - special case of low angle, high symmetry grain boundary. Most commonly, twinning corresponds to mirror symmetry around twinning plane.

coherent twin boundary

incoherent twin boundary (much higher energy)

good atomic fit at coherent twin boundary ⇒ low energy comparable to that of a stacking fault

Five degrees of freedom: 3 for the relative misorientation of the crystal and two for the direction of the grain boundary plane normal

Twist boundaries: axis of rotation of one crystal relative to the other is normal to the plane of the boundary

Tilt boundary: axis of rotation lies in the plane of the boundary

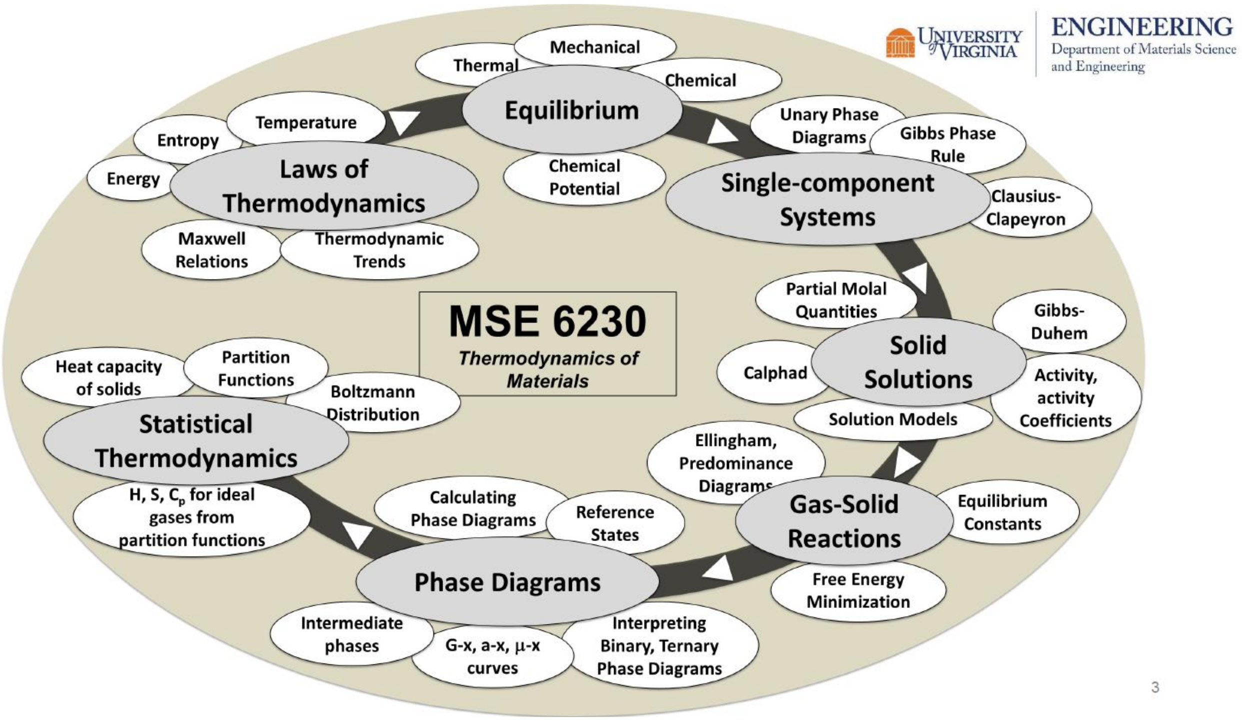
Coincidence site lattice(CSL)

1/Σ of the lattice points coincide

Singular GBs: low energy interface, low Σ

Defect textbook's summary can be helpful

Thermodynamics:



Basic law

State the basic laws for the thermodynamics? (include the 0th law)

State your understanding for entropy? Discuss the entropy with the system entropy, produced entropy, transfer entropy

Origin of entropy?

Configurational entropy, vibrational entropy, Electronic scale in terms of thermal excitation of electrons and spin polarizations, such as magnetic and ferroelectric polarizations.

Talk about the difference between reversible process and irreversible process.

Distinguish state function and process variable for thermodynamic quantity.

Classify the state function with Extensive and intensive state function.

How to understand enthalpy?

Bonding, energy in pressure, isobaric process

Why free energy is useful?

Easy to measure by fixing T,V or T,P

In Gibbs free energy, you can see PV is insensitive compare to TS term.

TS is more sensitive, so it's easy to change the mechanical properties by the heat treatment (processing)

(mechanical properties will change with temperature)

Sensitive→ the method to control the microstructure, to adjust

Insensitive→to protect something

Be familiar with the experimental variables: Coefficient of thermal expansion, Coefficient of compressibility, Heat capacity (specific heat)

Some quantity has absolute value, some may need reference state? Why is that and state your understanding about the reference state?

Derive all thermodynamic energy function and entropy with only heat capacity-temperature data.

Be familiar with the ideal gas related thermodynamic calculation. Equation of state and other specific experimental variable form.

Statistical thermodynamics:

State the aim of the statistical mechanics and how it connects to the phenomenology theory.

Connect micro- and Macro-

State the entropy related formula.

What's the partition function? Be familiar with how to derive other thermodynamic quantities based on partition function.

State the difference and similarities between different ensemble? (extra)

Phase diagram?

From unary/homogeneous to multicomponent/heterogeneous:

What's the chemical potential?

What's the Clausius-Clapeyron Eqn. ? How about the assumptions used in the P-T diagram with the C.-C. equation? For condensed phase, triple point especially. Note the graphical method used here with the approximation.

Slope in the P-T diagram

At least can reproduce the P-T diagram for water.

What's the partial molar properties?

What's the Gibbs-Duhem equation?

What's the mixing process?

Mixing is the formation of a solution from its own components (P,T constant) and results in a change of state for each component when forming a homogeneous solution.

State the method of Graphical Determination of PMPs?

What's the three types of equilibrium conditions for multicomponent systems?

Explain and discuss about the graphic thermodynamics? Check the notes on Zangari and Soffa's course. Graphical Determination of Partial molar properties.

What's the Gibbs-Duhem equation?

What's the partial molal properties?

What’s the activity? How it connects to the chemical potential?

Experimental measurements are not aimed however at chemical potential, but instead at activity,

$\Delta\mu_k = RTlna_k$ (effective concentration?)

$$a_k = \gamma_k X_k$$

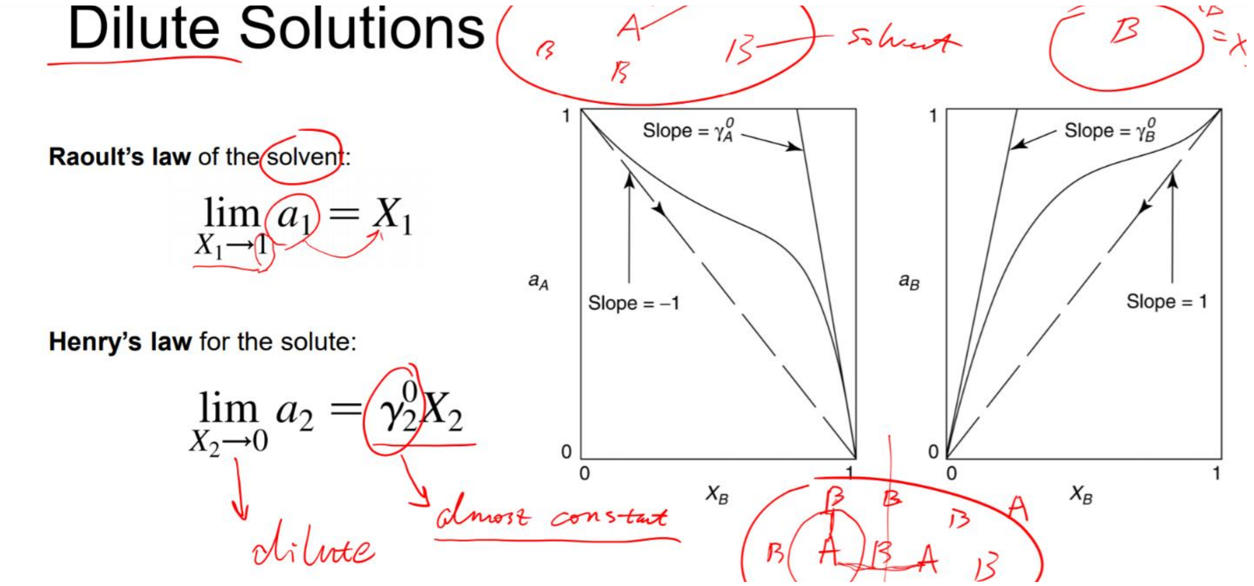
Ideal mixing: only ideal entropy produced by randomly distributed.

γ is an excess term.

fugacity (effective partial pressure)

What’s the dilute solution?

What’s the Henry’s law and Roult’s law? (Basically, a limit estimation)



Dilute Solutions

Raoult’s law of the solvent:

$$\lim_{X_1 \to 1} a_1 = X_1$$

Henry’s law for the solute:

$$\lim_{X_2 \to 0} a_2 = \gamma_2^0 X_2$$

dilute

almost constant

Mixing Problem: What’s the ideal mixing? What’s the regular mixing? What’s the subregular mixing? What’s the non-regular mixing? Quasi-chemical theory of mixing?

ideal mixing

only randomly distributed, entropy mixing, which is ideal mixing free energy

regular mixing

ideal mixing’s entropy+ mixing enthalpy (excess mixing Gibbs free energy) only related to composition simplest is $a_0 X_1 X_2$

subregular mixing

allows asymmetry in bond energy

non-regular mixing

consider T dependence

they are all about the excess mixing Gibbs free energy

Quasi-chemical theory of mixing

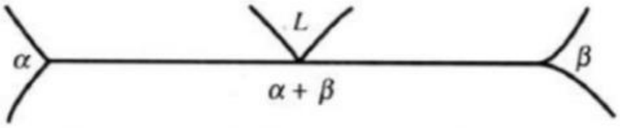
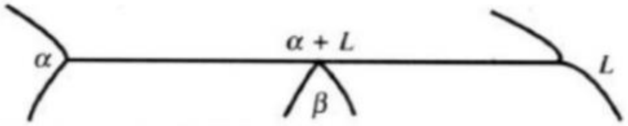
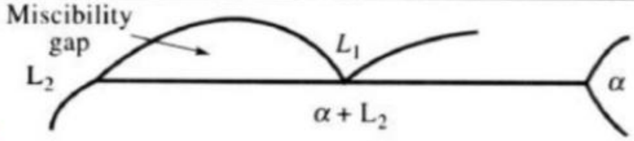
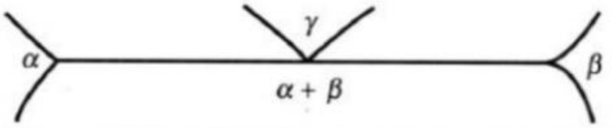
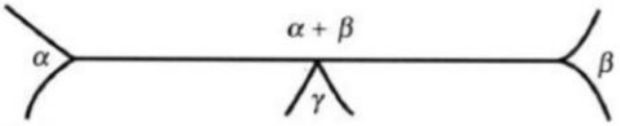
Consider bond energy statistically

Be famillar with the clustering vs. Ordering

What's the Eutectic, eutectoid, peritectic, monotectic, eutectoid, peritectoid?

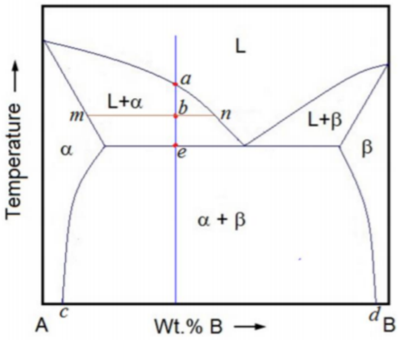
What's the pearlite?

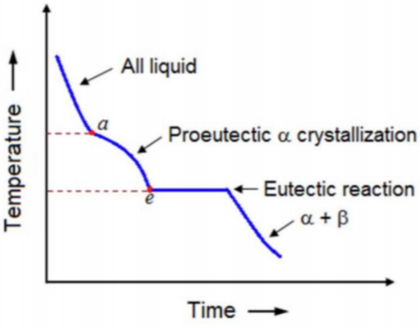
What's the hypoeutectoid, proeutectoid, hypereutectoid, hypoeutectic?

Eutectic	$L \rightarrow \alpha + \beta$	
Peritectic	$\alpha + L \rightarrow \beta$	
Monotectic	$L_1 \rightarrow L_2 + \alpha$ $\beta_1 \rightarrow \beta_2 + \alpha$	
Eutectoid	$\gamma \rightarrow \alpha + \beta$	
Peritectoid	$\alpha + \beta \rightarrow \gamma$	

Eutectic cooling

- While cooling a hypoeutectic alloy from the liquid state, the temp. drops continuously till liquidus point, *a*, at which crystals of proeutectic α begins to form.
- On further cooling the fraction of α increases. At any point, *b*, in the two-phase region the α fraction is given by the *lever rule* as *bn/mn*.





What’s the Lamellar Eutectic Structure?

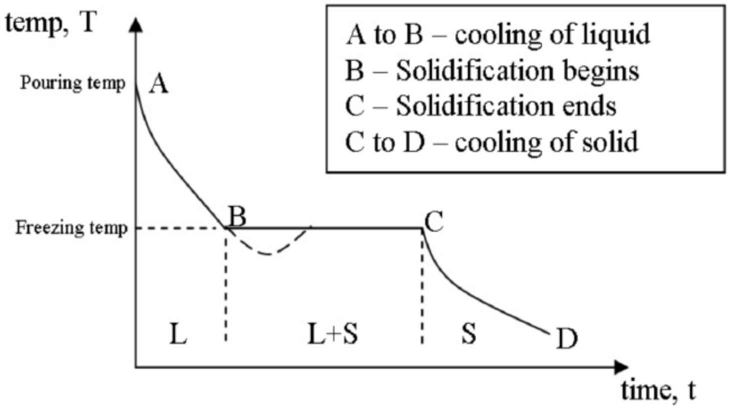
What’s the miscibility gap? What’s the spinodal decomposition? How to connect it to the graph?

How to connect the phase diagram to the G-X curve?

Cooling curve:

Cooling Curves during Solidification

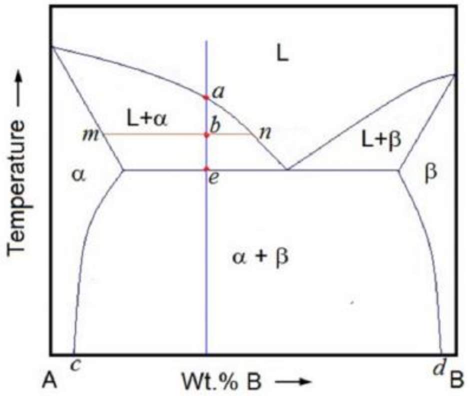
Experimental method to determine phase diagrams

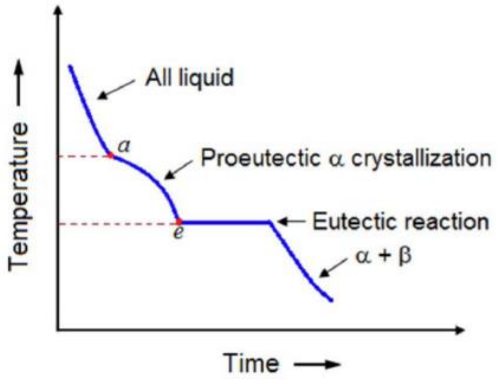


Solidification occurs at constant temperature while latent heat of fusion is released

Eutectic cooling

- While cooling a hypoeutectic alloy from the liquid state, the temp. drops continuously till liquidus point, *a*, at which crystals of proeutectic α begins to form.
- On further cooling the fraction of α increases. At any point, *b*, in the two-phase region the α fraction is given by the *lever rule* as *bn/mn*.





Reference state: The choice of reference state for each component must be the same, Be familiar with the standard reference state.

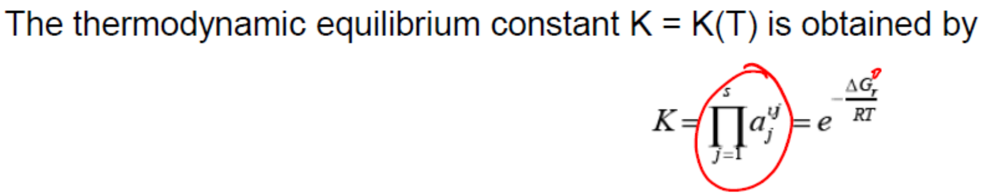
$G - H_{SER}$, the Gibbs energy relative to the enthalpy of the "Standard Element Reference" ie the reference phase for the element at 298.15 K

With the 3rd Law, Temperature and entropy and heat capacity has the absolute value, but the energy function basically doesn't has this. The only meaningful part of the energy is the energy difference which is actually the "driving force" or the "potential"

What's the heat of reaction?

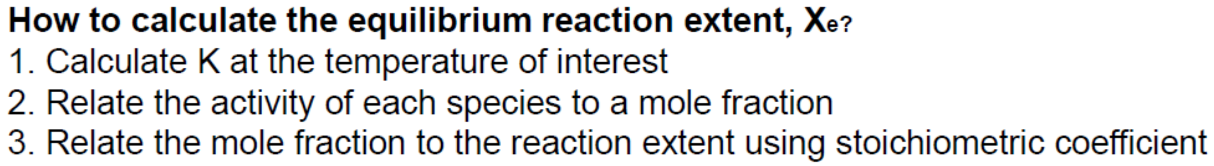
Heat of reaction = difference between the heat of formation of products and that of reactants

How reaction equilibrium constant connects to the free energy? Consider how it connect to the reaction rate with the reaction coefficient.



The thermodynamic equilibrium constant K = K(T) is obtained by

$$K = \prod_{j=1}^{s} a_j^{\nu_j} = e^{-\frac{\Delta G_r^0}{RT}}$$

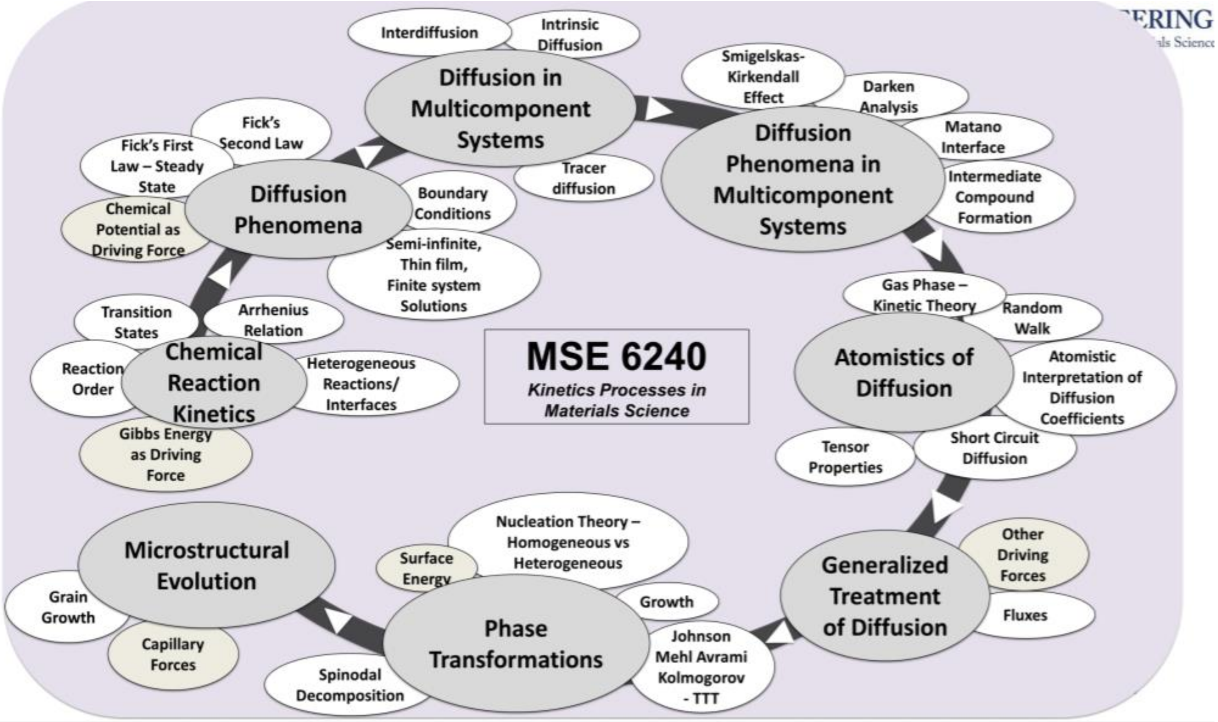


How to calculate the equilibrium reaction extent, X_e?

1. Calculate K at the temperature of interest
2. Relate the activity of each species to a mole fraction
3. Relate the mole fraction to the reaction extent using stoichiometric coefficient

Be familiar with the Ellingham diagrams, Predominance diagram and Pourbaix diagram.

Kinetics:



Chemical reaction kinetics

What is an equilibrium constant? What is a reaction rate constant? How do the forward and reverse reaction rate relate to equilibrium constant?

Diffusion phenomena

What's the flux for diffusion? The unit?

What's the driving force for steady-state diffusion?

What's Fick's 1st and 2nd law? State it clearly.

What's the unit for diffusion coefficient?

What's the feature of the steady-state diffusion?

what's the Arrhenius equation?

Recognize the different boundary condition for the diffusion?

What's the activation energy?

Diffusion in multicomponent systems

Discuss the Kirkendall diffusion couple experiment

Diffusion phenomena in multicomponent system

Atomistic diffusion

Derive the atomistic diffusion coefficient based on the random walk?

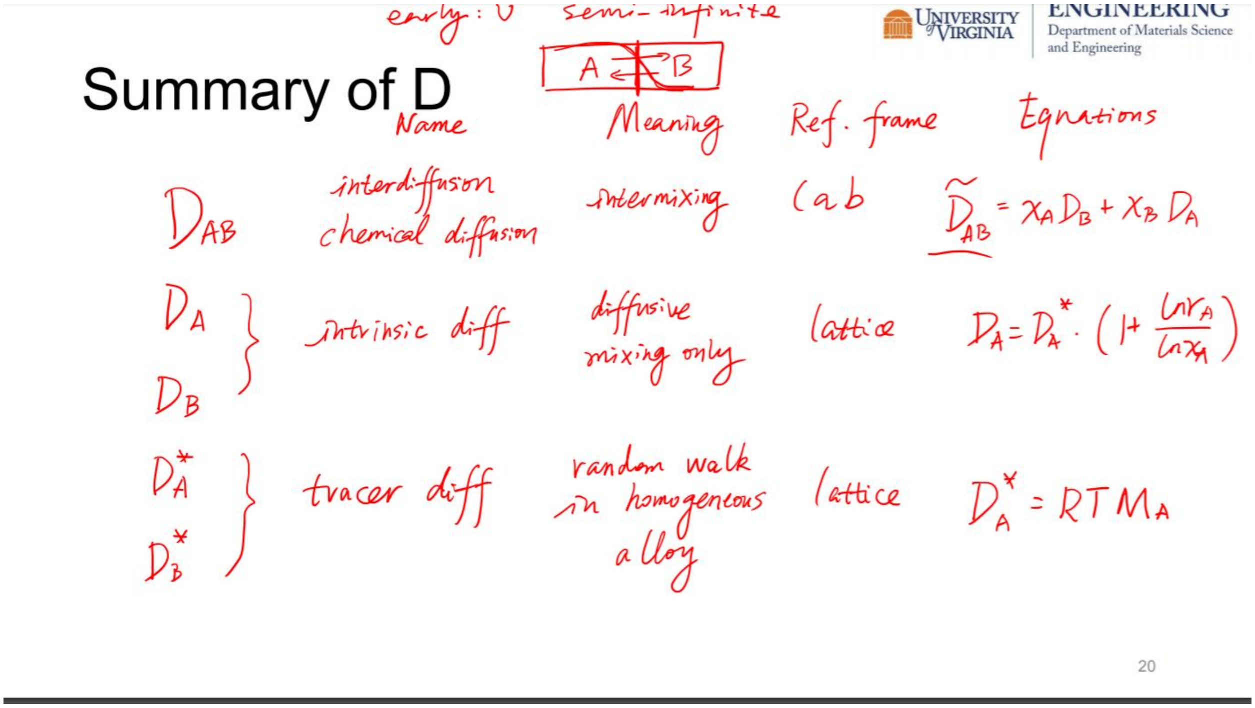
Illustrate different kinds of diffusion coefficient?

Self-diffusion coefficient

Interdiffusion coefficient

Intrinsic diffusion coefficient

Tracer diffusion coefficient



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Department of Materials Science and Engineering

early: U semi-infinite

Summary of D

	Name	Meaning	Ref. frame	Equations
D_{AB}	interdiffusion chemical diffusion	intermixing	lab	$\underline{\tilde{D}_{AB}} = x_A D_B + x_B D_A$
D_A D_B	intrinsic diff	diffusive mixing only	lattice	$D_A = D_A^* \cdot \left(1 + \frac{\ln \gamma_A}{\ln x_A}\right)$
D_A^* D_B^*	tracer diff	random walk in homogeneous alloy	lattice	$D_A^* = RTM_A$

Rank diffusion coefficient for diffusion with defects?

The larger free volume, the larger diffusion coefficient.

Similar question: diffusion mechanism, interstitial is faster, as its activation energy is smaller

Heterogeneous nucleation, energy barrier.

Generalized treatment of diffusion

Phase transformations

What are the two typical rate controlling steps in passive oxidation?

Explain the meaning of the nucleation theory, homogeneous and heterogeneous?

What's the spinodal decomposition?

What's the surface energy? Based on free energy and enthalpy. It also appears in the defects class for free surface. Lecture 22 interface.

Coherent: large strain energy, small chemical energy

Incoherent: small strain energy, large chemical energy

May be incorrect

The chemical energy + structure energy means interface energy

Incoherent has dominated structure energy (not strain energy) and less chemical energy

Interface energy for coherent is mostly chemical energy

Interfacial vs. strain energy

The strain energy involved depends on the type of interfaces between the nucleus and the matrix:

a. Coherent interfaces: lattice planes and directions are continuous across the interface. High strain energy and low interfacial energy ($\gamma_{coh} \approx 0.01 - 0.1\, J/m^2$).

b. Incoherent interfaces: there is no correspondence of line or planes across the interface. Materials can slid along such an interface and the interface can transmit normal stress, but not shear stress. Low strain energy and high interfacial energy ($\gamma_{incoh} \approx 0.5\, J/m^2$).

c. Semicoherent interfaces: They have local lattice correspondence. The interface contains misfit dislocations.

Interfacial energy: $\gamma_{coh} < \gamma_{semi} < \gamma_{incoh}$

Strain energy: $\Delta G_{coh} > \Delta G_{semi} > \Delta G_{incoh}$

competition between elastic energy and interfacial energy can result is a sequence of precipitation reactions ⇒ appearance of successively more stable precipitates, each of which has a larger nucleation barrier

Example: in Al alloys with 5% Cu (maximum solid solubility of Cu in Al at T_e

The sequence is $\alpha_0 \rightarrow \alpha_1 + \text{GP-zones} \rightarrow \alpha_2 + \theta" \rightarrow \alpha_3 + \theta' \rightarrow \alpha_4 + \theta$

α_n - fcc aluminum; n^{th} subscript denotes each equilibrium

GP zones - mono-atomic layers of Cu on $(001)_{Al}$

θ" - thin discs, fully coherent with matrix

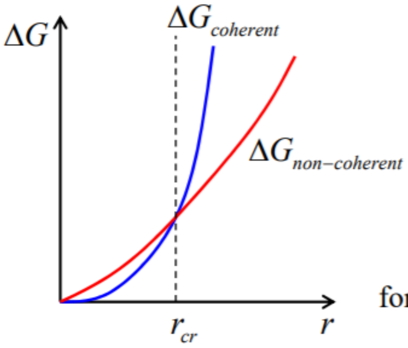
θ' - disc-shaped, semi-coherent on $(001)_{\theta'}$ bct

θ - incoherent interface, ~spherical, complex body-centered tetragonal (bct)

The precipitate with the smallest nucleation barrier (generally) appears first. Small nucleation barriers are associated with coherent interfaces (small interfacial energy) and similar lattices (small elastic energies from misfit).

competition of volumetric elastic strain energy and interfacial energy ⇒ precipitate may start as fully coherent but nucleate interfacial dislocations once it reaches a critical size

Assuming that elastic strain energy is significant for the fully coherent precipitate but not for incoherent or semicoherent ones, the free energies of crystals with coherent and non-coherent precipitates can be written as



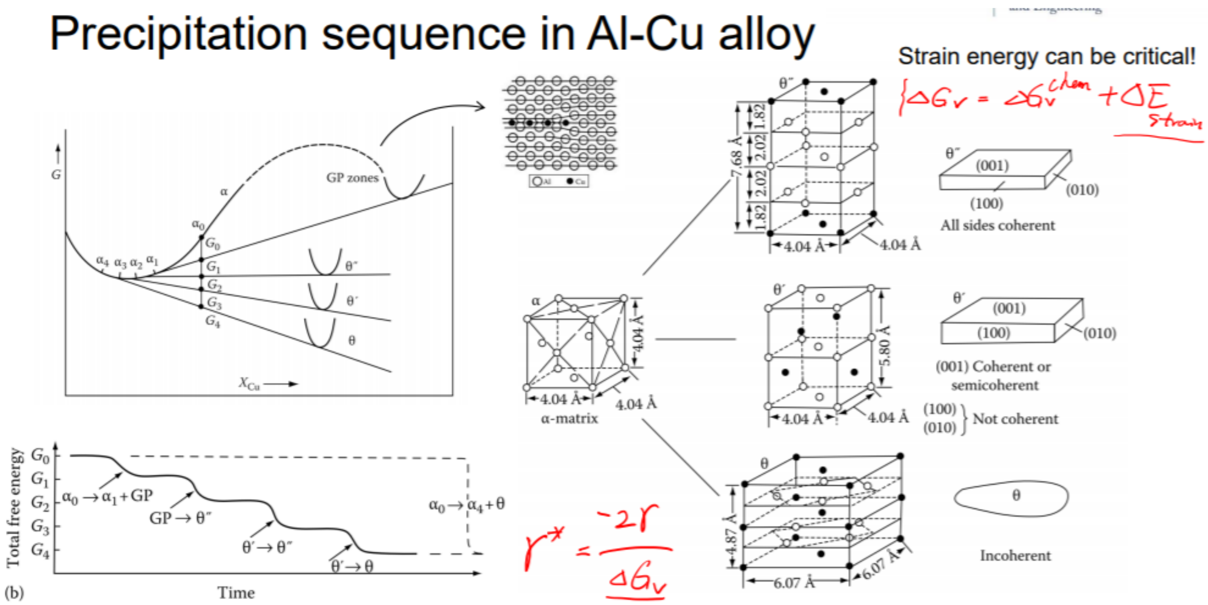
$$\Delta G_{coherent} = \Delta G_{elastic} + \Delta G_{\text{interface}} = 4G\delta^2 \times \frac{4}{3}\pi r^3 + \gamma_{chem} \times 4\pi r^2$$

$$\Delta G_{non-coherent} = \Delta G_{elastic} + \Delta G_{\text{interface}} = 0 + \left(\gamma_{chem} + \gamma_{str}\right) \times 4\pi r^2$$

$$\Delta G_{coherent} = \Delta G_{non-coherent} \quad \Longrightarrow \quad r_{cr} = \frac{3\gamma_{st}}{4G\delta^2}$$

for semicoherent interfaces with large D: $\gamma_{st} \sim \delta \quad \Longrightarrow \quad r_{cr} \sim \frac{1}{\delta}$

at $r > r_{cr}$, dislocations can be nucleated ⇒ the character of the interface will change ⇒ coherency will be lost

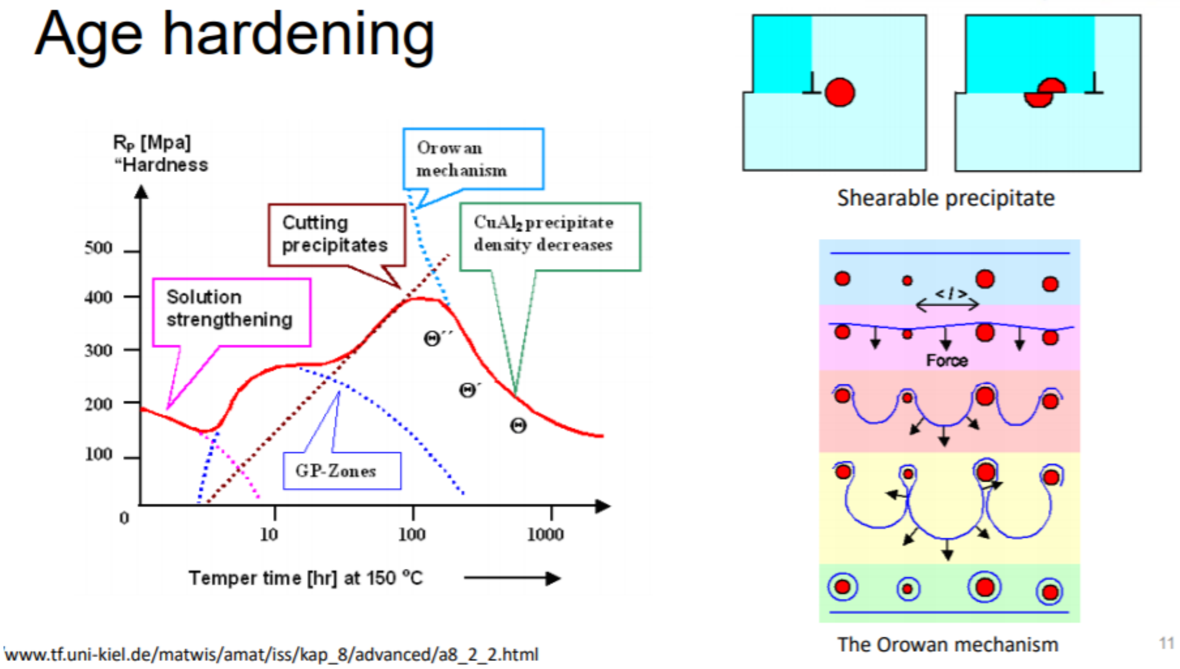


Precipitation sequence in Al-Cu alloy

Strain energy can be critical!

$\{\Delta G_v = \Delta G_v^{chem} + \Delta E_{strain}$

$r^* = \frac{-2\gamma}{\Delta G_v}$



Age hardening

Shearable precipitate

The Orowan mechanism

www.tf.uni-kiel.de/matwis/amat/iss/kap_8/advanced/a8_2_2.html

Explain the shape of the TTT diagram?

WHAT'S THE DIFFERENCE BETWEEN CCT/TTT diagram?

CCT consider the non-equilibrium case in the real case, so it will shift the TTT diagram a little bit, As TTT consider the isothermal reaction only, which is the ideal situation.

Capillary force? Driving force for it?

What's the coarsening? Gibbs–Thomson effect?

Grain growth? Why it exists?

Reduce surface area to reduce the boundary energy

Reduce energy for the whole crystal.

Microstructural evolution

What's the capillary effect?

Application sides:

structure materials and mechanical properties

what's the stress and strain? What's the yielding?

What's the Poisson ratio? How it connects the modulus constants in different directions?

What's the engineering stress-strain behavior? Indicate: modulus of elasticity, Yielding, proportional limit, Yield strength, Tensile strength, necking, fracture?

Compare stress-strain and other behavior for the eternal field and internal response, BH curve, polarization and electric field.

Bonus: how to compare it with magnetic hysteresis curve?

Mathematical understanding: eternal field and response

Why first linear then non-linear?

Derivative and small perturbation.

Irreversible thermodynamics provide linear Onsager reciprocal relations

What's the Ductility? How to quantify it?

What's the resilience? And toughness?

Indicate the difference between engineering stress-strain and true stress-strain?

Cross sectional area will decrease

Talk about the ductile strength trade off?

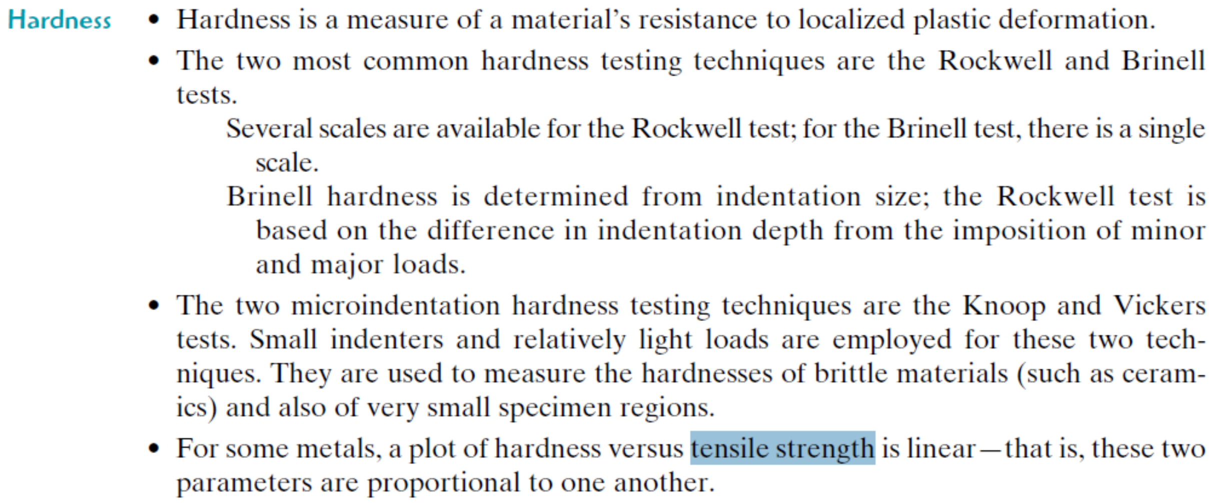
What other trade off?

Example: Hall-Petch effect and its inverse?

Nucleation's volume contribution and surface contribution/ TTT/CCT C-curve nucleation growth C-curve.

Which means you have to balance

What's the hardness?



Hardness

- Hardness is a measure of a material's resistance to localized plastic deformation.
- The two most common hardness testing techniques are the Rockwell and Brinell tests.
  - Several scales are available for the Rockwell test; for the Brinell test, there is a single scale.
  - Brinell hardness is determined from indentation size; the Rockwell test is based on the difference in indentation depth from the imposition of minor and major loads.
- The two microindentation hardness testing techniques are the Knoop and Vickers tests. Small indenters and relatively light loads are employed for these two techniques. They are used to measure the hardnesses of brittle materials (such as ceramics) and also of very small specimen regions.
- For some metals, a plot of hardness versus tensile strength is linear—that is, these two parameters are proportional to one another.

why we study dislocation for the mechanical properties?

Dislocation motion and plastic deformation.

What's the slip system?

How to strength the materials? And what's the common strengthening mechanism?

Switching Gears:
Strengthening Mechanisms

The ability to plastically deform a material depends on the ease of dislocation movement…

So you can strengthen a material by impeding this motion!!!!

=> Materials engineers can strengthen crystals by a variety of means:

Grain Size Reduction

Solution Strengthening

Strain Hardening (Cold Work)

Precipitation Strengthening (We wont discuss)

Strain hardening=cold work=Taylor hardening

Precipitation strengthening=dispersion hardening=age hardening~~~Orowan mechanism

What's the dislocation density? Two ways

What's the recover, recrystallization, grain growth?(see also Agnew's slides)

Recover

- There is some relief of internal strain energy by dislocation motion.

- Dislocation density decreases, and dislocations assume low-energy configurations.
- Some material properties revert back to their precold-worked values.

recrystallization

- A new set of strain-free and equiaxed grains form that have relatively low dislocation densities.
- The metal becomes softer, weaker, and more ductile.
- temperature increases (at constant heat-treating time), tensile strength decreases and ductility increases
- Plastic deformation of a metal above its recrystallization temperature is *hot working*; deformation below its recrystallization temperature is termed *cold working*.

Grain growth is the increase in average grain size of polycrystalline materials, which proceeds by grain boundary motion.

What's their driving force for recrystallization, grain growth? And what's their feature?

Phase transformation and materials processing:

Are you familiar with the lever rule? Make sure you can work out it within ternary system as well.

State the invariant reaction and the meaning for it?

-oid: solid only reaction

Eutectic reaction, Peritectic reaction

What's the Eutectic, eutectoid, peritectic, monotectic, eutectoid, peritectoid?

What's the pearlite?

What's the hypoeutectoid, proeutectoid, hypereutectoid, hypoeutectic?

What kind of special structure will form during the eutectic reaction?

Iron-carbon phase diagram:

Pearlite: lamellar

Cementite: Fe3C

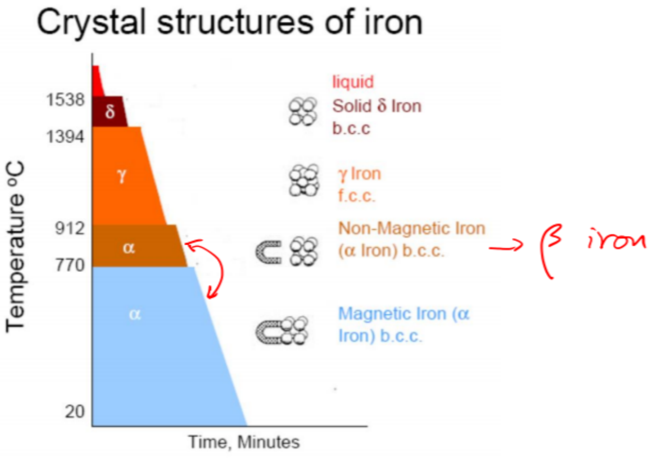
Austenite:

ferrite

martensite:

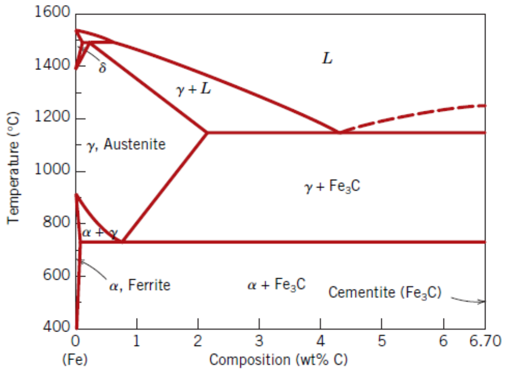
Iron-Carbon System

- Pure iron when heated experiences 2 changes in crystal structure before it melts.
- At room temperature the stable form, ferrite (α iron) has a BCC crystal structure.
- Ferrite experiences a polymorphic transformation to FCC austenite (γ iron) at 912 ˚C (1674 ˚F).
- At 1394˚C (2541˚F) austenite reverts back to BCC phase δ ferrite and melts at 1538 ˚C (2800 ˚F).
- Iron carbide (cementite or Fe_3C) an intermediate compound is formed at 6.7 wt% C.
- Typically, all steels and cast irons have carbon contents less than 6.7 wt% C.
- Carbon is an interstitial impurity in iron and forms a solid solution with the α, γ, δ phases.



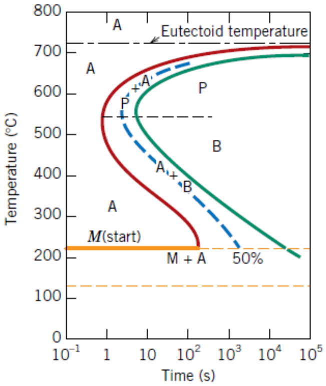
Crystal structures of iron

Iron–Carbon Alloys
(Steels)
(Processing)



Iron–iron carbide phase diagram
(Chapter 9)

→



Isothermal transformation diagrams
(Chapter 10)

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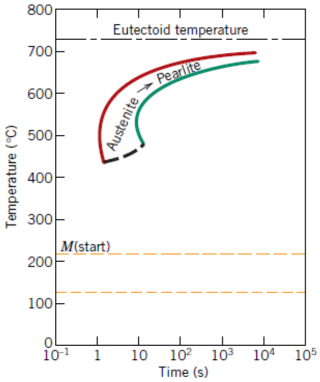

Continuous-cooling transformation diagrams
(Chapter 10)

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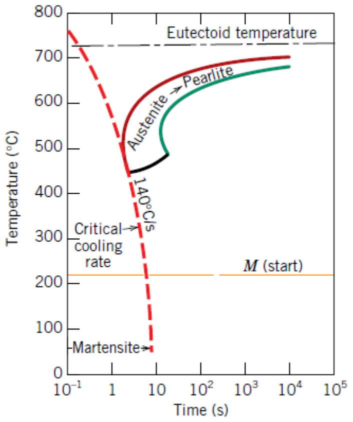
Martensite (formation of)
(Chapter 10)



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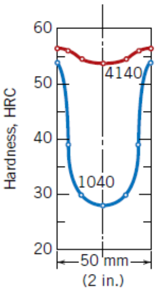
Tempering (tempered martensite)
(Chapter 10)

martensite (BCT, single phase) →

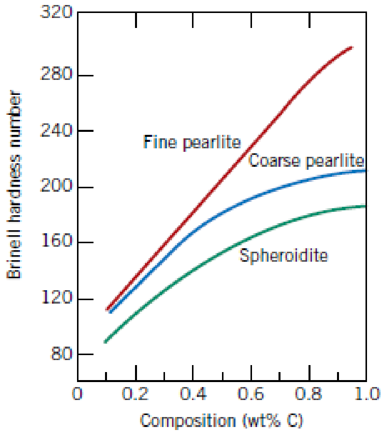
tempered martensite (α + Fe_3C phases)

→

Heat treatment of steels
(Chapter 11)



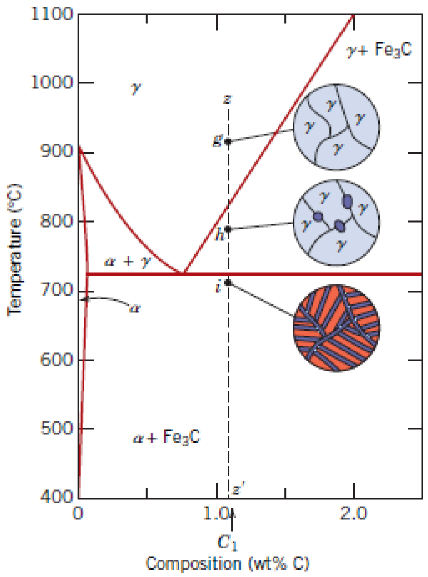
Structure **Properties**



Development of microstructure in iron–carbon alloys
(Chapters 9 & 10)

Mechanical properties of iron–carbon alloys
(Chapter 10)

- **Pearlite (coarse and fine)**
- **Bainite**
- **Spheroidite**
- **Martensite**
- **Tempered martensite**



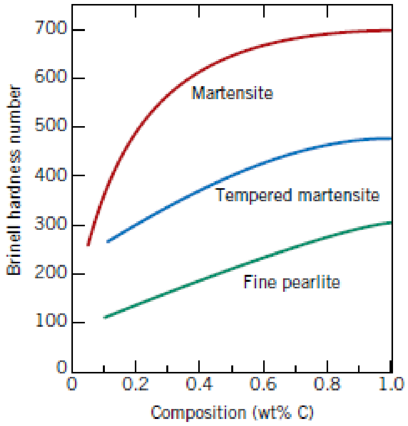


Table 10.2 Microstructures and Mechanical Properties for Iron–Carbon Alloys

Microconstituent	*Phases Present*	*Arrangement of Phases*	*Mechanical Properties (Relative)*
Spheroidite	α-Ferrite + Fe_3C	Relatively small Fe_3C spherelike particles in an α-ferrite matrix	Soft and ductile
Coarse pearlite	α-Ferrite + Fe_3C	Alternating layers of α-ferrite and Fe_3C that are relatively thick	Harder and stronger than spheroidite, but not as ductile as spheroidite
Fine pearlite	α-Ferrite + Fe_3C	Alternating layers of α-ferrite and Fe_3C that are relatively thin	Harder and stronger than coarse pearlite, but not as ductile as coarse pearlite
Bainite	α-Ferrite + Fe_3C	Very fine and elongated particles of Fe_3C in an α-ferrite matrix	Harder and stronger than fine pearlite; less hard than martensite; more ductile than martensite
Tempered martensite	α-Ferrite + Fe_3C	Very small Fe_3C spherelike particles in an α-ferrite matrix	Strong; not as hard as martensite, but much more ductile than martensite
Martensite	Body-centered, tetragonal, single phase	Needle-shaped grains	Very hard and very brittle

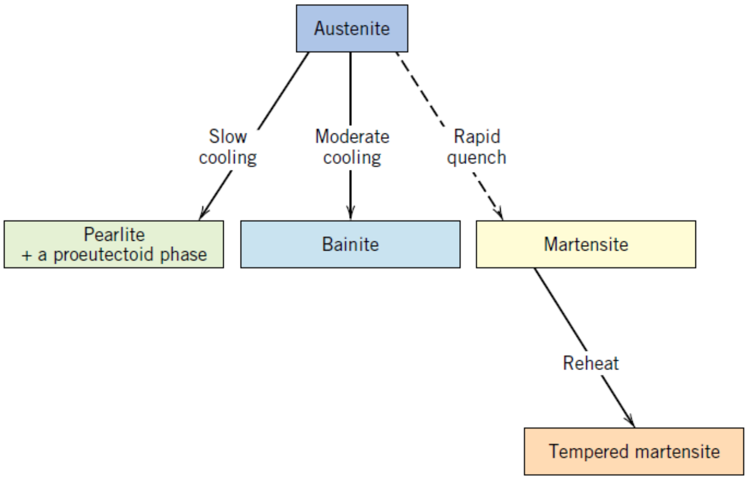
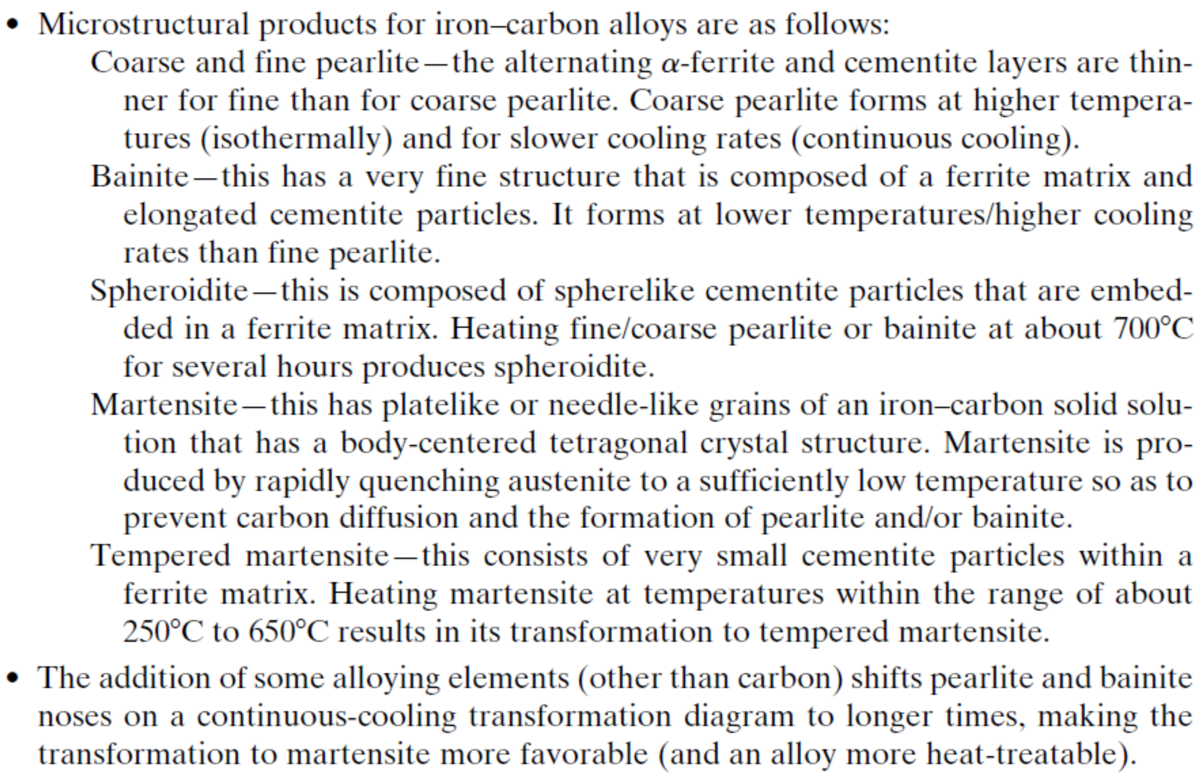
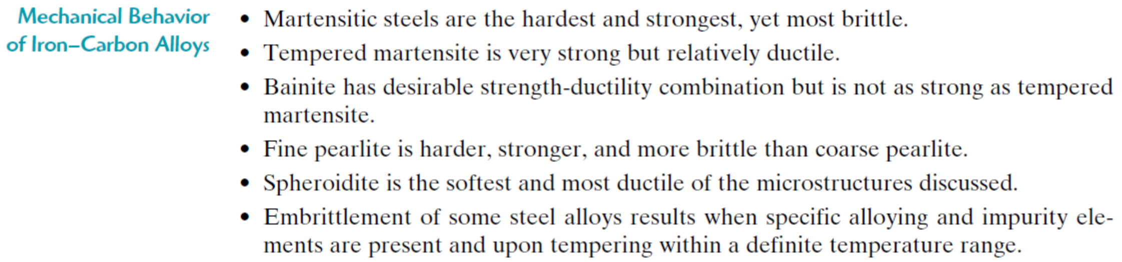


Figure 10.36 Possible transformations involving the decomposition of austenite. Solid arrows, transformations involving diffusion; dashed arrow, diffusionless transformation.



- Microstructural products for iron–carbon alloys are as follows:
  - Coarse and fine pearlite—the alternating α-ferrite and cementite layers are thinner for fine than for coarse pearlite. Coarse pearlite forms at higher temperatures (isothermally) and for slower cooling rates (continuous cooling).
  - Bainite—this has a very fine structure that is composed of a ferrite matrix and elongated cementite particles. It forms at lower temperatures/higher cooling rates than fine pearlite.
  - Spheroidite—this is composed of spherelike cementite particles that are embedded in a ferrite matrix. Heating fine/coarse pearlite or bainite at about 700°C for several hours produces spheroidite.
  - Martensite—this has platelike or needle-like grains of an iron–carbon solid solution that has a body-centered tetragonal crystal structure. Martensite is produced by rapidly quenching austenite to a sufficiently low temperature so as to prevent carbon diffusion and the formation of pearlite and/or bainite.
  - Tempered martensite—this consists of very small cementite particles within a ferrite matrix. Heating martensite at temperatures within the range of about 250°C to 650°C results in its transformation to tempered martensite.
- The addition of some alloying elements (other than carbon) shifts pearlite and bainite noses on a continuous-cooling transformation diagram to longer times, making the transformation to martensite more favorable (and an alloy more heat-treatable).



Mechanical Behavior of Iron–Carbon Alloys

- Martensitic steels are the hardest and strongest, yet most brittle.
- Tempered martensite is very strong but relatively ductile.
- Bainite has desirable strength-ductility combination but is not as strong as tempered martensite.
- Fine pearlite is harder, stronger, and more brittle than coarse pearlite.
- Spheroidite is the softest and most ductile of the microstructures discussed.
- Embrittlement of some steel alloys results when specific alloying and impurity elements are present and upon tempering within a definite temperature range.

Describe the Gibbs phase rule?

What’s the two main phase transformation method?

spinodal decomposition:

nucleation and growth:

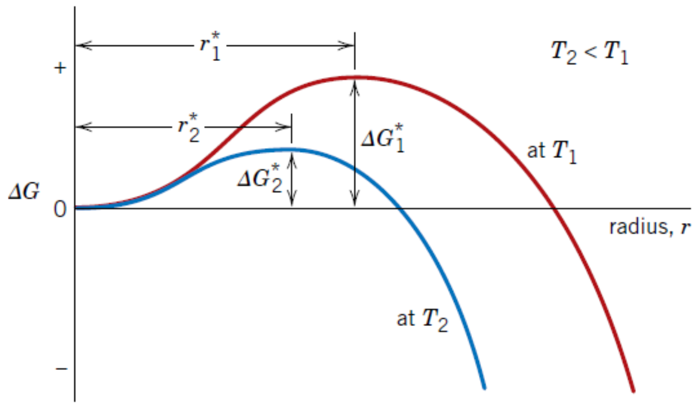


Figure 10.3 Schematic free energy-versus-embryo/nucleus-radius curves for two different temperatures. The critical free energy change (ΔG^*) and critical nucleus radius (r^*) are indicated for each temperature.

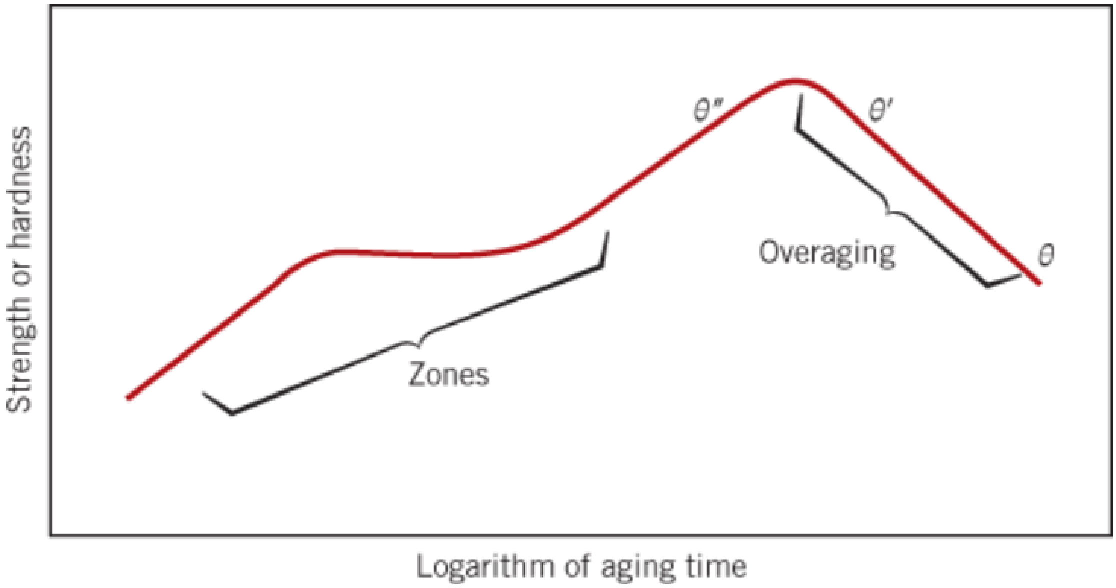
What’s the martensite phase?

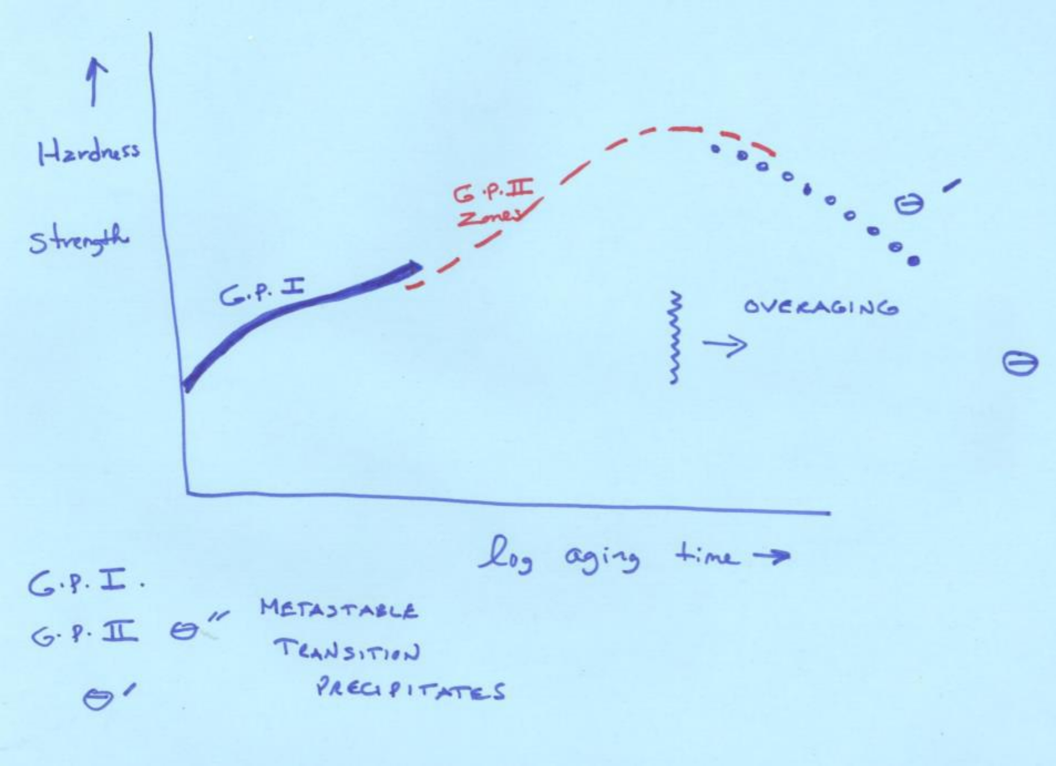
What’s the precipitation? And G.P. zone?

What’s the annealing and casting?

What’s the overaging?

Talk about the strength-time relation during the precipitation hardening?




Hardness
Strength
G.P. I
G.P. II
Zones
θ'
OVERAGING
θ
log aging time →
G.P. I.
G.P. II θ''
METASTABLE
TRANSITION
PRECIPITATES
θ'