

Mechanical Behavior of Materials

Lec.02-06

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This recitation class will cover lecture 2 to 6, the topics include:

- Bonding in Solids & Crystalline Structures (Lec.2)
- Crystallographic Directions/Planes and Defects (Lec.3)
- Physics of Elastic and Inelastic Deformation (Lec.4)
- Phase Diagrams (Lec.5&6)

Agenda

- 1 Bonding in Solids
- 2 Crystallographic Basics
- 3 Defects
- 4 Physics of Elastic and Inelastic Deformation
- 5 Phase Diagrams

Types of Interatomic Bonds

Primary Bonds

- Ionic Bonds: electron transfer
- Covalent Bonds: electron sharing
- Metallic Bonds: electron cloud

Secondary Bonds

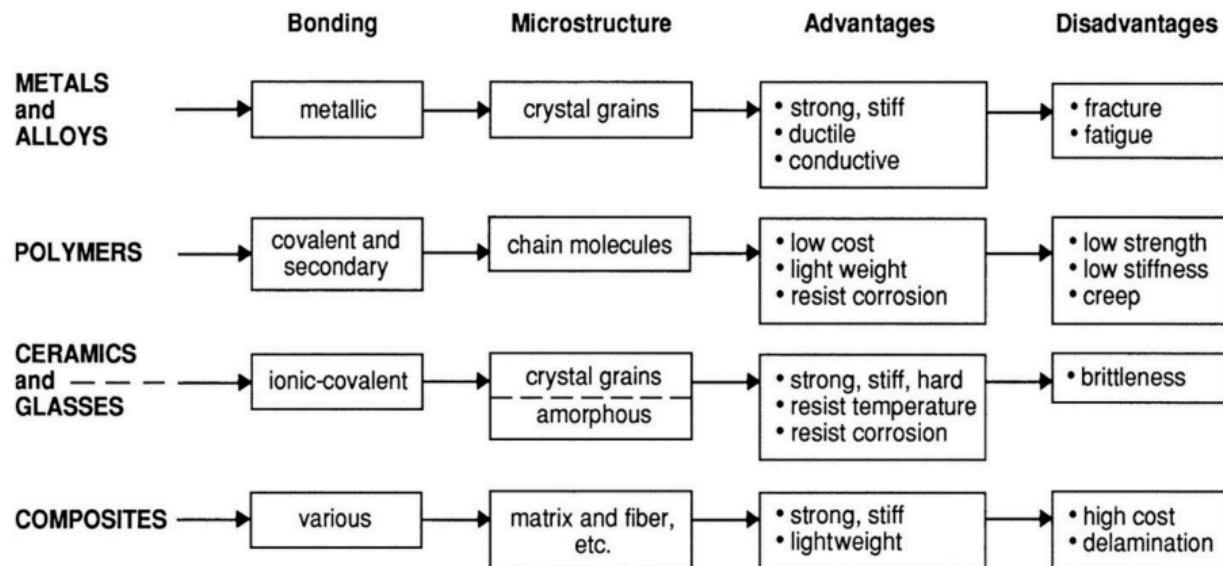
- Van der Waals Bonds: dipole-dipole, dipole-induced dipole, and dispersion forces
- Hydrogen Bonds: special case of dipole-dipole interaction

Types of Interatomic Bonds

Type	Bond Energy	Comment
Ionic	Large	Non-directional, high T_m and E
Covalent	Large	Directional, high T_m and E
Metallic	Variable	Non-directional, moderate T_m and E
Van der Waals	Small	Non-directional, low T_m and E
Hydrogen	Small	Directional, low T_m and E

Types of Materials

Materials can be classified by the type of dominant bonding present between the atoms.



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Crystal Structures



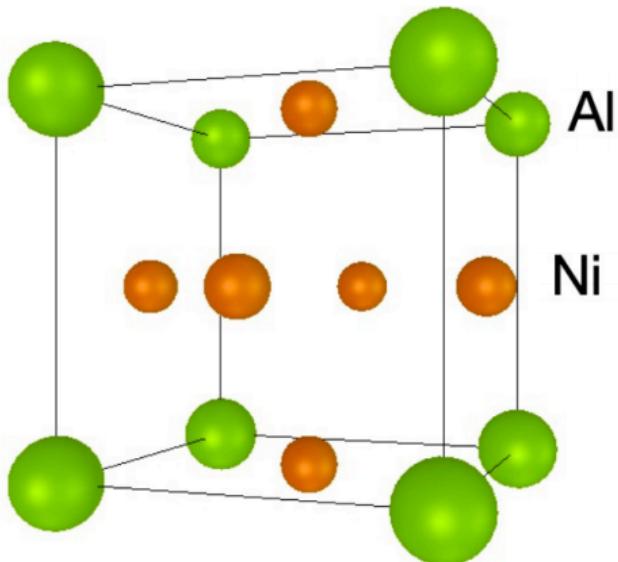
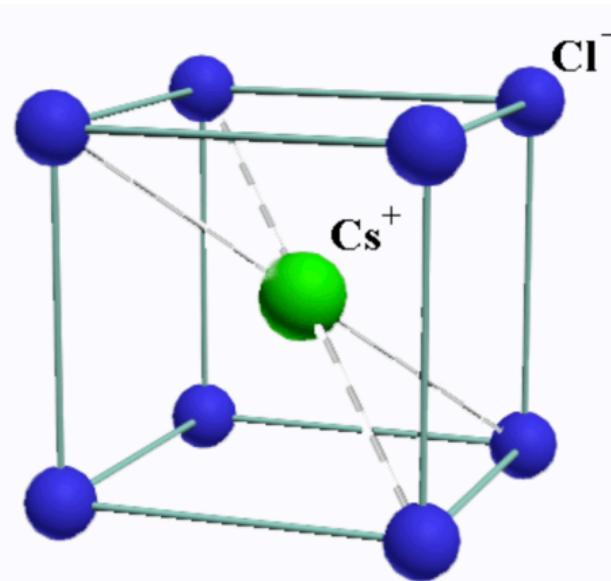
Crystal structure = Lattice structure + Basis

- Lattice describes the repetition pattern or periodicity, or intrinsically, the translational symmetry of the crystal.
- Basis describes the motif, i.e. the detailed atom arrangement, at each lattice point

Crystal Structures

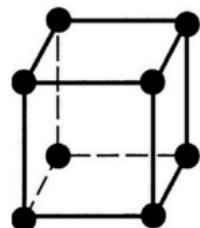
Example

What is the lattice and basis of the following crystal structure?

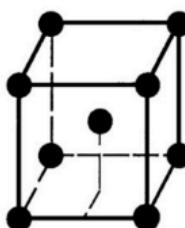


Unit Cell

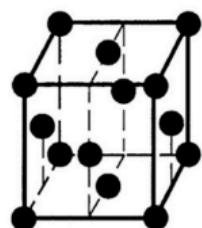
Primitive-cubic Body-centered-cubic Face-centered-cubic Hexagonal-close-packed
or simple cubic



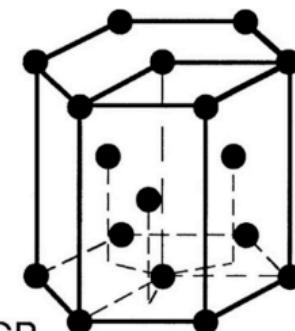
PC



BCC



FCC



HCP

- Unit Cell is a simple unit of a crystal, which could generate the whole crystal if repeated.
- Unit cell contains information about chemistry (basis) and symmetry (lattice structure).
- Choice of unit cell is not unique.

Crystallographic Directions

Definition

A crystallographic direction is a line between two points in a crystal, which is described by a vector.

Crystallographic directions are specified by three integers enclosed in square brackets $[uvw]$. The algorithm is as follows:

- ① Vector is repositioned (if necessary) to pass through the origin.
- ② Read off line projections (to principal axes of unit cell) in terms of fractional of unit cell dimensions a , b , and c
- ③ Adjust to smallest integer values
- ④ Enclose in square brackets, no commas

Crystallographic Planes

Definition

A Miller index is a series of coprime integers that are inversely proportional to the intercepts of the crystallographic planes with the edges of the unit cell.

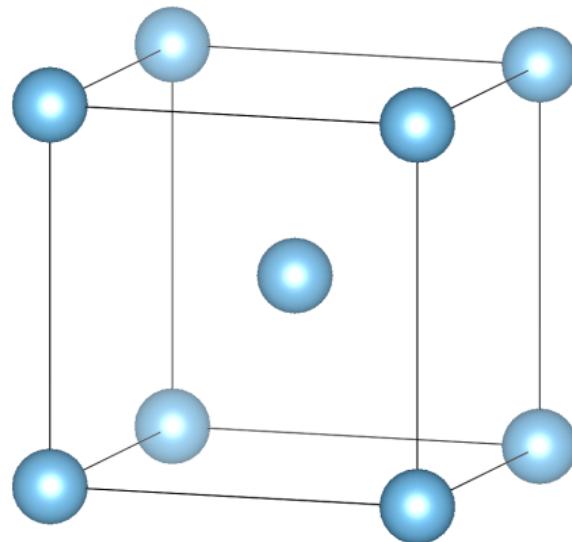
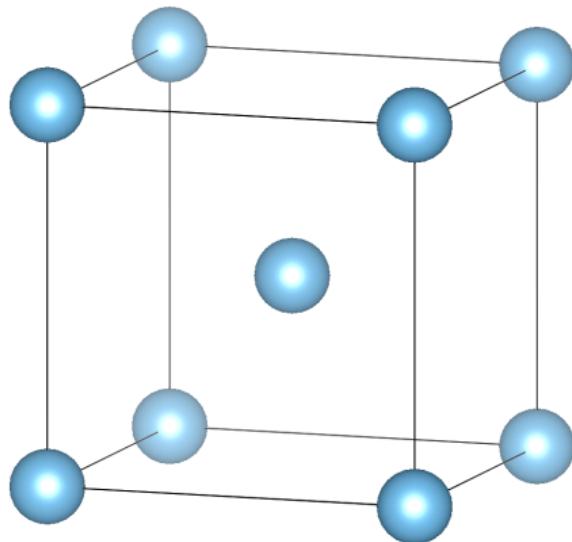
Crystallographic planes are specified by three Miller indices as (hkl) . The algorithm is as follows:

- ① Read off intercepts of plane with axes in terms of a , b , c
- ② Take reciprocals of intercepts
- ③ Reduce to smallest integer values
- ④ Enclose in parentheses, no commas i.e., (hkl)

Crystalllographic Directions & Planes

Example

Sketch crystallographic directions and planes in the BCC unit cell below.

 $\langle 33\bar{2} \rangle$  $(33\bar{2})$

Density Calculation

Linear Density

$$\text{Linear Density} = \frac{\text{Number of atoms}}{\text{Unit length of direction vector}}$$

Planar Density

$$\text{Planar Density} = \frac{\text{Number of atoms}}{\text{Area of 2D repeat unit}}$$

Theoretical Density

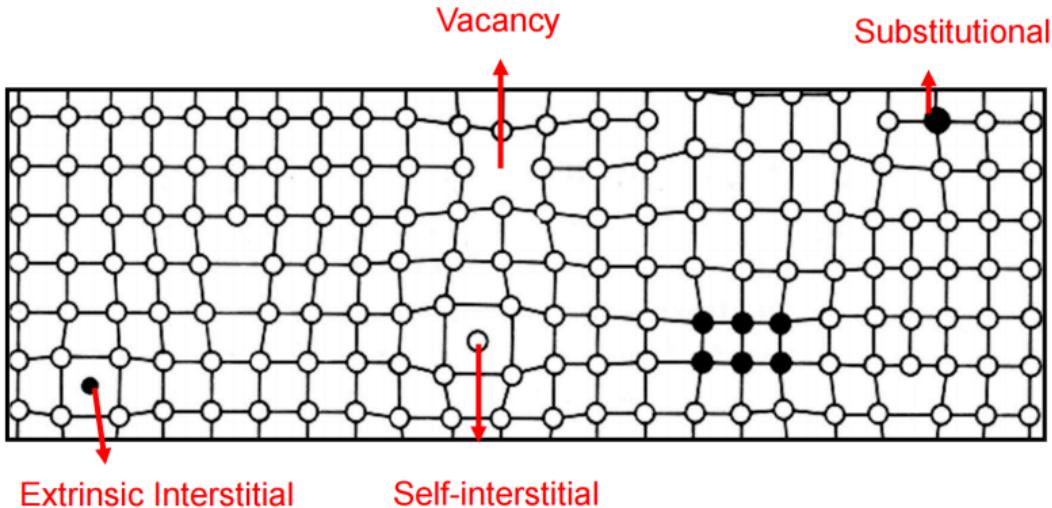
$$\rho = \frac{nA}{V_C N_A}$$

n is the number of atoms per unit cell, A is the atomic weight, V_C is the volume of the unit cell, and N_A is Avogadro's number.

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Point Defects



- Vacancy is unoccupied lattice site
- Interstitial impurity occupies position between lattice sites
- Substitutional impurity occupies normal lattice site

Equilibrium Concentration of Vacancies

In a crystal containing N atomic sites, the number of vacancies N_v is:

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

- A is a proportionality constant
- Q_v is the energy required to create a vacancy
- k is the Boltzmann constant
- T is the temperature

Point Defects in Alloy

Two outcomes if impurity (B) added to host (A):

- Solid solution of B in A
 - Substitutional solid solution: sites of the solvent metal are occupied by solute metal atoms.
 - Interstitial solid solution: the solute atoms occupy holes (interstices) within the solvent metal structure.
- Solid solution of B in A plus particles of a new phase
 - Intermetallic compound: some mixtures of metals form alloys with definite structures that may be unrelated to the structures of each of the individual metals.

Hume-Rothery Rules

Criteria for substitutional solid solution:

- Similar atomic radius with $\Delta r < 15\%$
- Similar electronegativities
- Same crystal structure for pure metals
- Given the same conditions, a metal will have a greater tendency to dissolve a metal of higher valency than one of lower valency

Line Defects

Definition

Line defects are called dislocations and are the edges of surfaces where there is a relative displacement of lattice planes.

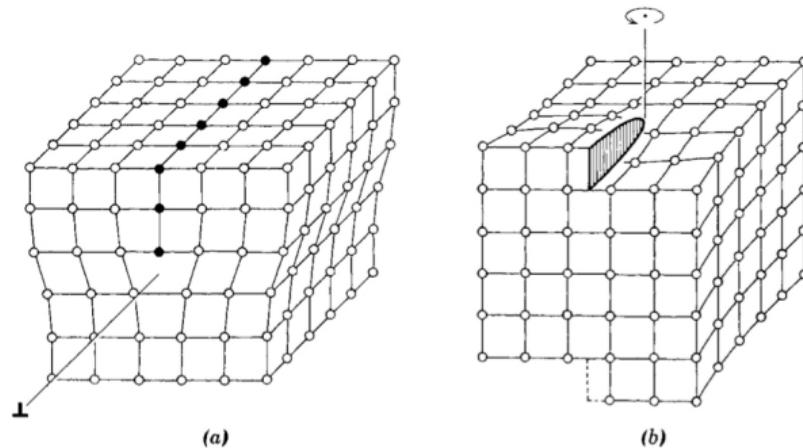
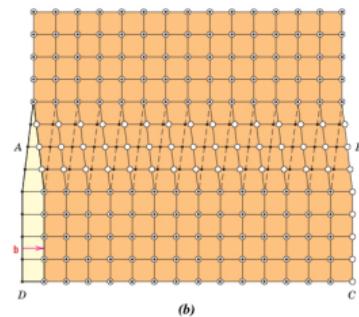
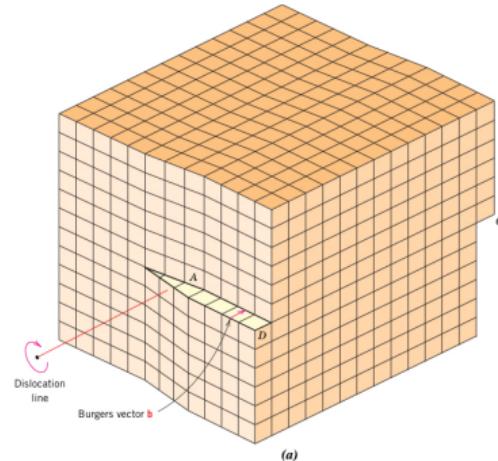
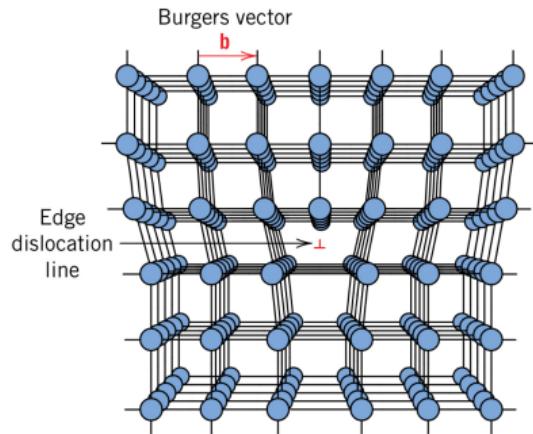


Figure 2.14 The two basic types of dislocations: (a) edge dislocation, and (b) screw dislocation. (From [Hayden 65] p. 63; used with permission.)

Mechanical properties of materials are closely related to dislocation motion.

Dislocation Line & Burgers Vector



Dislocation Line & Burgers Vector

Type	Description
Edge	\vec{b} is perpendicular to the dislocation line
Screw	\vec{b} is parallel to the dislocation line
Mixed	\vec{b} has both edge and screw components

Definition

\vec{b} is the Burgers vector, which characterizes the magnitude and direction of the lattice distortion associated with the dislocation.

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Interatomic Force

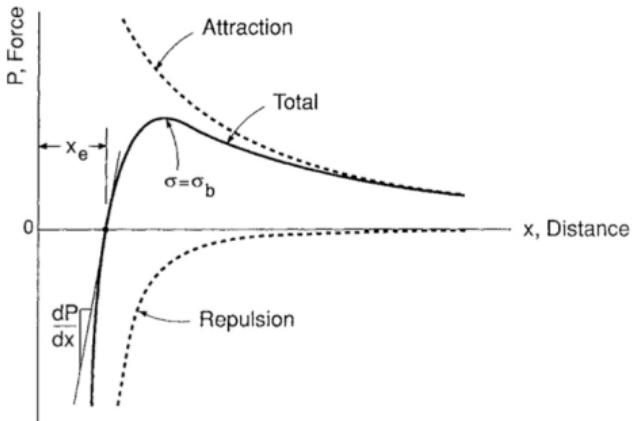


Figure 2.16 Variation with distance of the attractive, repulsive, and total forces between atoms. The slope dP/dx at the equilibrium spacing x_e is proportional to the elastic modulus E ; the stress σ_b , corresponding to the peak in total force, is the theoretical cohesive strength.

- Total force is attractive at large distance, repulsive at short distance, and zero at equilibrium atomic spacing x_e .
- Elastic deformation represent a small perturbation about x_e .

Elastic Deformation

Definition

Elastic deformation is macroscopic view of accumulation of inter-atomic distance changes through out the material, which recovers immediately when external stress removed.

The difficulty of elastic deformation is characterized by the elastic modulus:

$$E = \frac{d\sigma}{d\epsilon} \Big|_{x=x_e} = \frac{x_e}{A} \frac{dP}{dx} \Big|_{x=x_e}$$

- E is the intrinsic property of materials dominated by the bonding of the materials. Microstructure and defects do not affect E .
- Strong primary bonds are resistant to stretching and so result in high value of E (Typically, metal \approx ceramic $>$ polymer).
- As T rises, bonds are easier to separate from equilibrium spacing, so E decreases.
- E is isotropic for polycrystalline materials, but anisotropic for single crystals.

Plastic Deformation

Definition

Deformation that does not disappear when the stress is removed is called plastic deformation.

- Plastic deformation occurs mainly by shear.
- Theoretical shearing through breaking all the atomic bonds between two layers at the same time.

$$\tau_b = \frac{Gb}{2\pi h} \approx \frac{G}{10} \quad \text{where } G = \frac{d\tau}{d\gamma}$$

- Actual shearing through slip. Discrepancy exists between theoretical and actual strength:
 - Actual ultimate tensile strength smaller than theoretical cohesive tensile strength $\sigma_b \approx \frac{E}{10}$ by factor of 10 to 100
 - Actual shear strength smaller than theoretical shear strength $\tau_b \approx \frac{G}{10}$ by factor of 300 to 10000

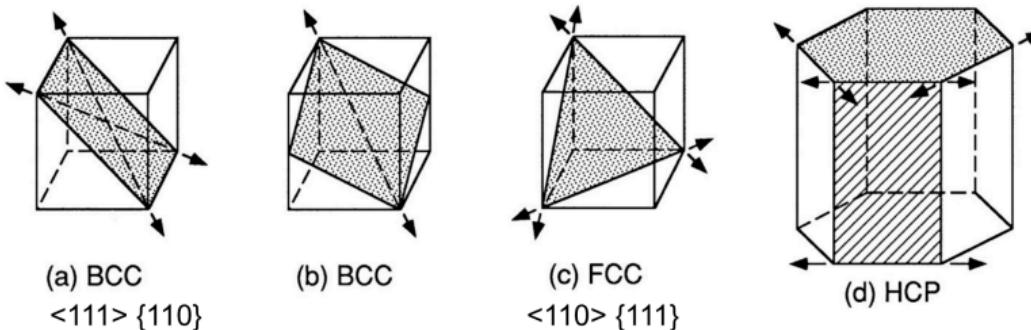
Slip Planes and Directions

Definition

The motion of dislocations in response to an externally applied shear stress is termed slip.

Slips are most likely occur along high atomic density plane and direction:

- Slip planes: close-packed planes
- Slip directions: close-packed directions
- Slip systems: combination of slip planes and directions, i.e. $\langle uvw \rangle \{ hkl \}$

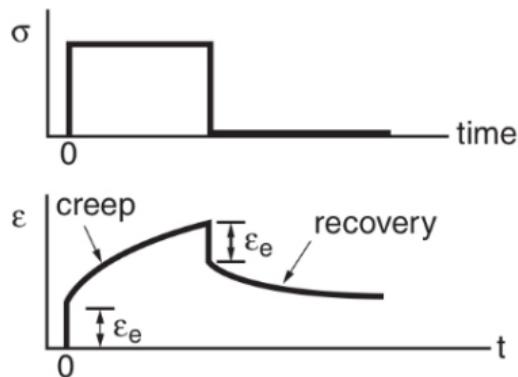


Dislocation and Hardening Mechanisms

If there are **obstacles** that impede dislocation motion, the strength of the material increases. Hardening mechanisms include:

- Strain hardening: **dislocation** density increases with plastic deformation, which increases the resistance to further deformation.
- Solid solution hardening: **impurity atoms** distort the lattice, which increases the resistance to dislocation motion.
- Precipitation hardening: **precipitates** impede dislocation motion.
- Grain size reduction: **grain boundaries** impede dislocation motion.

Creep Deformation



- Accumulation of creep strain with time under constant stress, and partial recovery after the removal of stress
- In crystals, caused by
 - Diffusional flow of vacancies
 - Grain boundary sliding, cavities forming
- In amorphous and in polymers, caused by
 - Chainlike molecule slide past one another (at $T > T_g$)

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Concepts & Terminology

Definition

Phase: A homogeneous portion of a system that has uniform physical and chemical characteristics.

- Dependent variables: T , P , Composition.
- Difference in either physical or chemical properties is sufficient to distinguish phases.
- Criteria for phase equilibrium: Gibbs free energy minimized, and there is no further tendency for change.

Concepts & Terminology

Definition

Component is the elements or compounds which are mixed initially.

- An alloy is described by stating the components and their concentration
- A binary alloy could be in the form of: (a) Single solid solution; (b) Two separated pure components; (c) Two separated solid solutions; (d) A chemical compound with a solid solution

Definition

Constitution is described by the phases present, weight fraction of each phase, and the composition of each phase.

Gibbs Phase Rule

$$P + F = C + N$$

- P : Number of phases present
- F : Number of degrees of freedom m or number of independent intensive variables that can be varied simultaneously and arbitrarily without affecting constitution (# of phases, what phases)
- C : Number of components
- N : Number of noncompositional variables (T, P)

Binary Phase Diagrams Calculation

Given a binary phase diagram, the composition of an alloy, its temperature, and assuming the system is at equilibrium, we can determine:

- **What phase(s) is (are) present**

- Locate the $T\text{-}C$ point on the phase diagram and notes the phases with which the corresponding phase field is labeled.

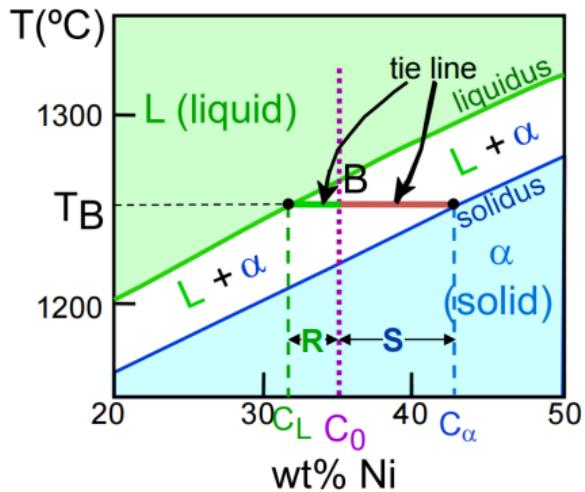
- **The composition(s) of the phase(s)**

- For single-phase regions, the composition of the phase is the same as the overall composition of the alloy.
 - For two-phase regions, construct a tie line through the $T\text{-}C$ point and intresect the phase boundary.

- **The mass fraction(s) of the phase(s)**

- For single-phase regions, the mass fraction of the phase is 1.
 - For two-phase regions, the mass fraction is determined by the lever rule.

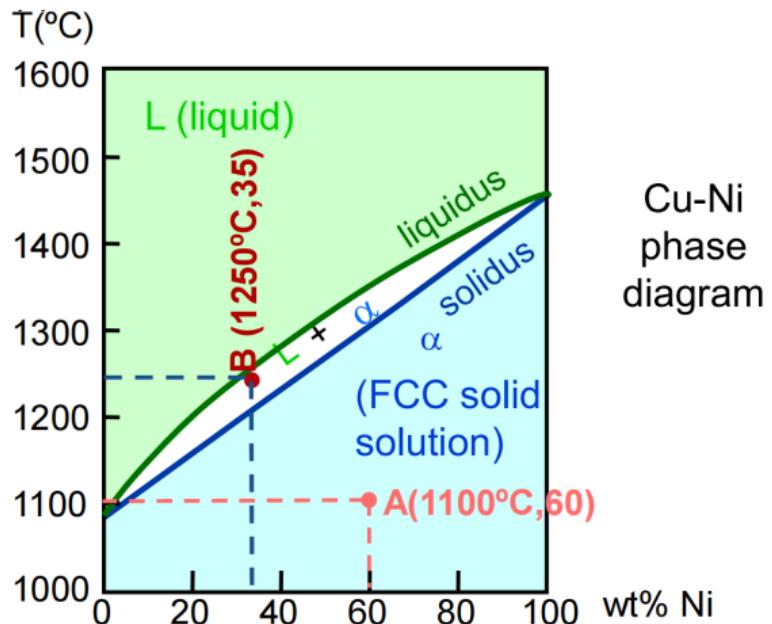
Lever Rule



$$W_L = \frac{S}{R+S} = \frac{C_\alpha - C_0}{C_\alpha - C_L} \quad W_\alpha = \frac{R}{R+S} = \frac{C_0 - C_L}{C_\alpha - C_L}$$

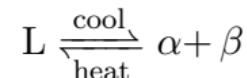
Binary Isomorphous System

Complete solubility of one component in another in liquid phase as well as solid phase.

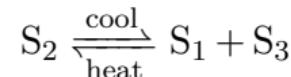


Eutectic, Eutectoid, & Peritectic

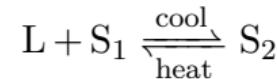
- Eutectic - liquid transforms to two solid phases



- Eutectoid - one solid phase transforms to two other solid phases

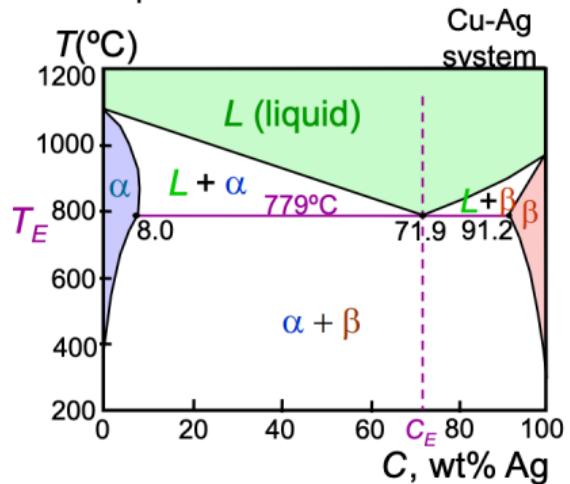


- Peritectic - liquid and one solid phase transform to a second solid



Binary Eutectic System

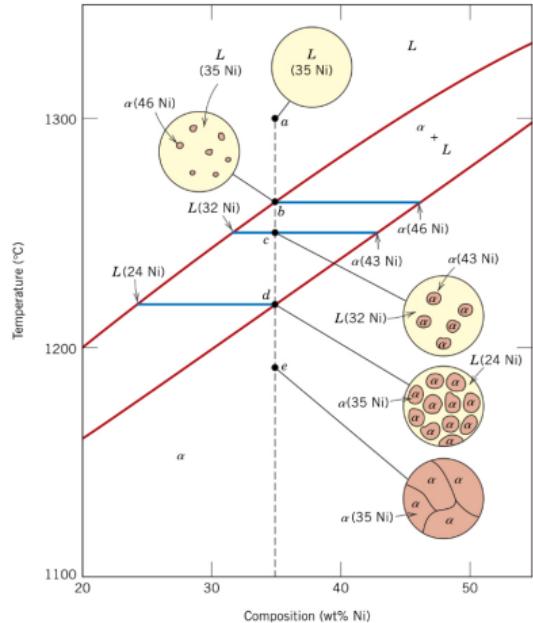
Complete solubility of one component in another in liquid phase but with limited solubility of one component in another in solid state.



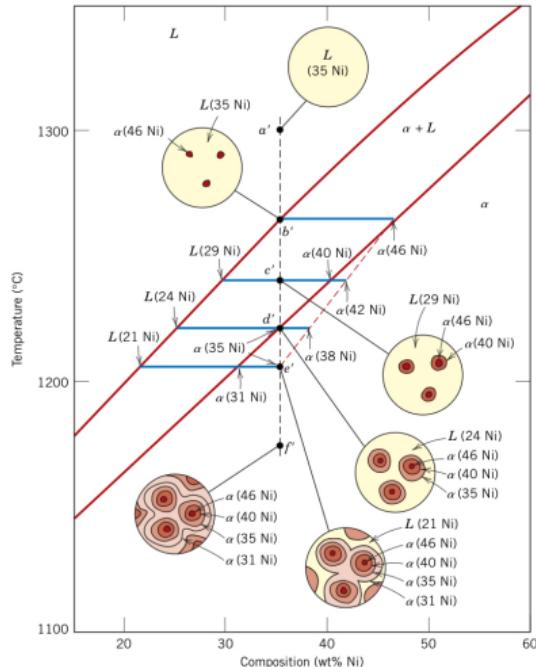
- 3 single phase regions (L, α, β)
- Eutectic reaction: $L(C_E) \rightarrow \alpha(C_{\alpha E}) + \beta(C_{\beta E})$
- Eutectic point: C_E, T_E

Development of Microstructure

For binary isomorphous system, the microstructure development is as follows:



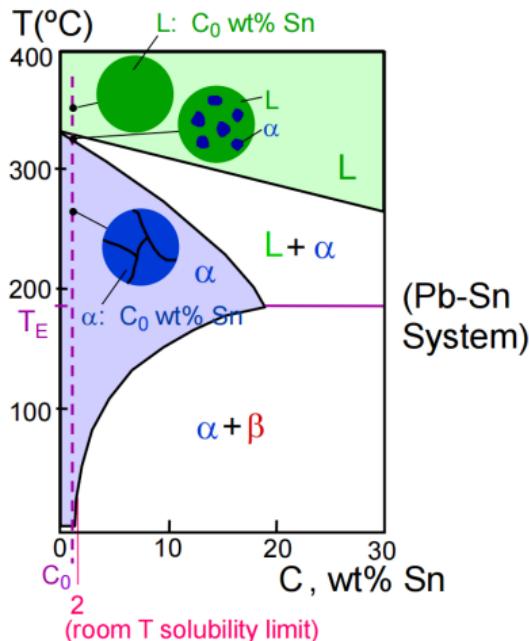
Equilibrium cooling



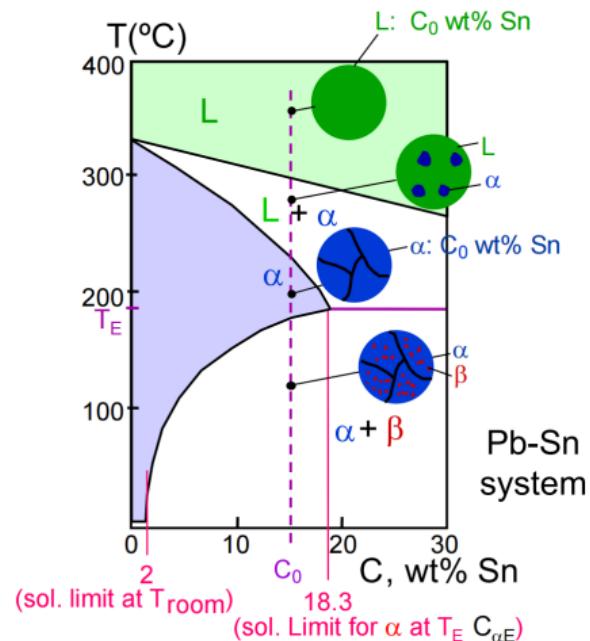
Nonequilibrium cooling

Development of Microstructure

For binary eutectic system, the microstructure development is as follows:



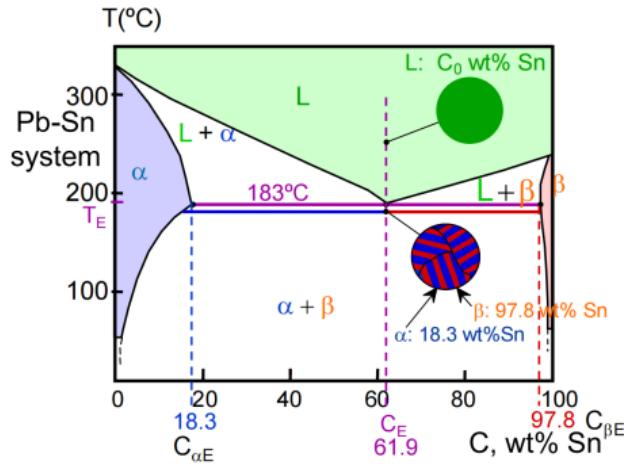
1. Below RT solubility limit



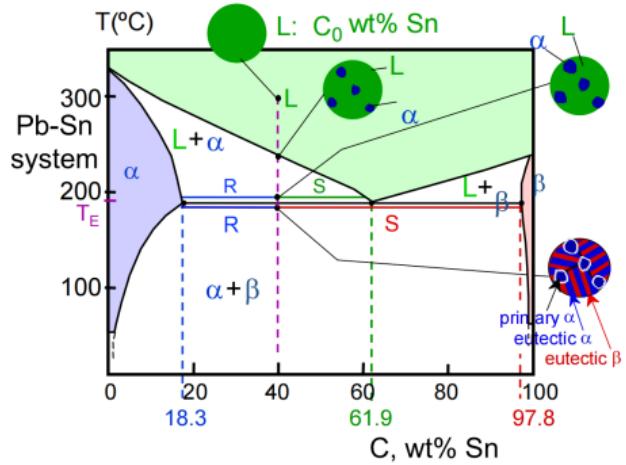
2. Between solubility limit at RT and T_E

Development of Microstructure

Continued:



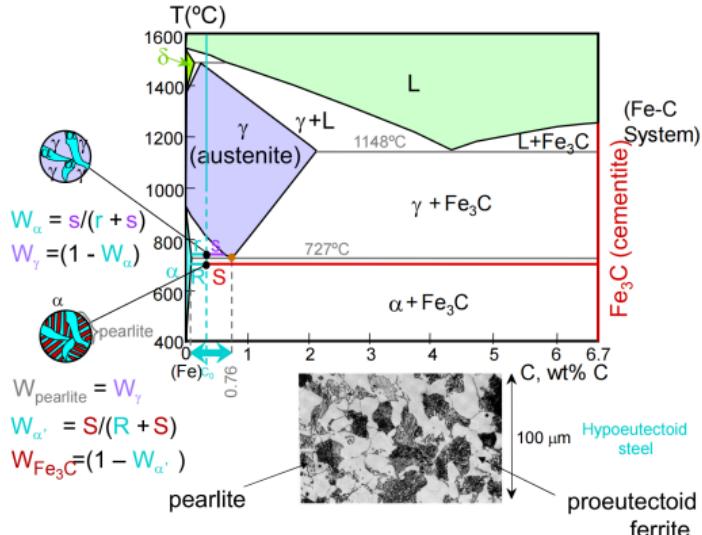
3. At C_E



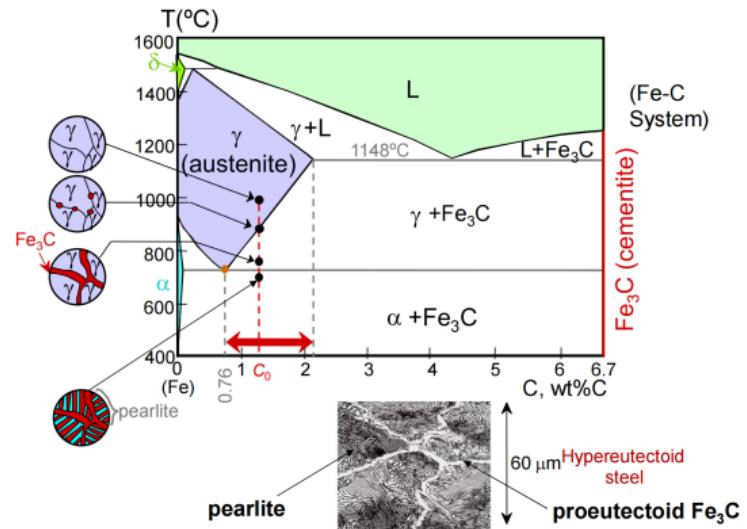
4. Other points on eutectic line except C_E

Development of Microstructure

For Iron-Carbon (Fe-C) system, the microstructure development is as follows:



Hypoeutectoid Steel



Hypereutectoid Steel

Example

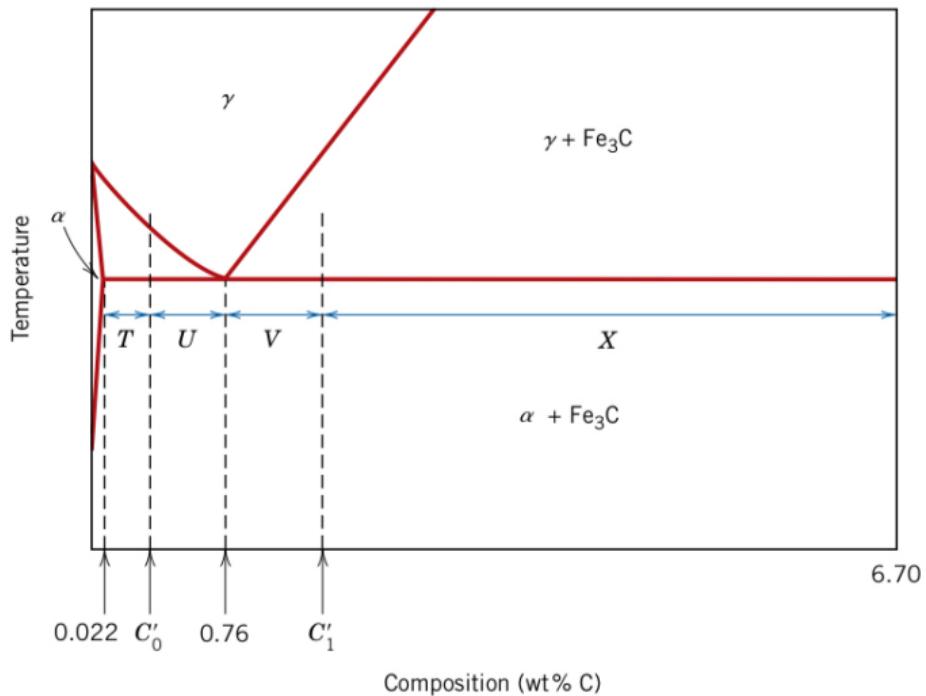
Example

For a 99.65 wt% Fe-0.35 wt% C alloy at a temperature just below the eutectoid, determine the following:

- (a) The fractions of total ferrite and cementite phases
- (b) The fractions of the proeutectoid ferrite and pearlite
- (c) The fraction of eutectoid ferrite

Example

For your reference:



Solution

(a) The fractions of total ferrite and cementite phases

(a) This part of the problem is solved by applying the lever rule expressions using a tie line that extends all the way across the $\alpha + \text{Fe}_3\text{C}$ phase field. Thus, C'_0 is 0.35 wt% C, and

$$W_{\alpha} = \frac{6.70 - 0.35}{6.70 - 0.022} = 0.95$$

and

$$W_{\text{Fe}_3\text{C}} = \frac{0.35 - 0.022}{6.70 - 0.022} = 0.05$$

Solution

(b) The fractions of the proeutectoid ferrite and pearlite

(b) The fractions of proeutectoid ferrite and pearlite are determined by using the lever rule and a tie line that extends only to the eutectoid composition (i.e., Equations 9.20 and 9.21). We have

$$W_p = \frac{0.35 - 0.022}{0.76 - 0.022} = 0.44$$

and

$$W_{\alpha'} = \frac{0.76 - 0.35}{0.76 - 0.022} = 0.56$$

Solution

(c) The fraction of eutectoid ferrite

(c) All ferrite is either as proeutectoid or eutectoid (in the pearlite). Therefore, the sum of these two ferrite fractions equals the fraction of total ferrite; that is,

$$W_{\alpha'} + W_{ae} = W_{\alpha}$$

where W_{ae} denotes the fraction of the total alloy that is eutectoid ferrite. Values for W_{α} and $W_{\alpha'}$ were determined in parts (a) and (b) as 0.95 and 0.56, respectively. Therefore,

$$W_{ae} = W_{\alpha} - W_{\alpha'} = 0.95 - 0.56 = 0.39$$

Thank you!