# ME5005/ME4002
# DESIGN FOR MANUFACTURE
# PRODUCTION ENGINEERING

Dr. Bill Wright
bill.wright@ucc.ie
Room 2.14 Tel: 490 2213

Lecture 3: Structure of Materials II



## Crystal imperfections

- Most materials contain imperfections in the atomic arrangement/lattice
- These defects often intentionally introduced to control mechanical and physical properties
  - Alloying
  - Heat Treatment
  - Processing
- Three main types:
  - Line DEFECTS (DISLOCATIONS)
  - Point DEFECTS
  - Surface DEFECTS



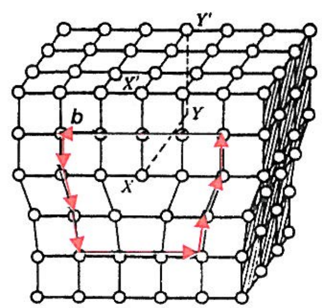
## Line defects (dislocations)

- Group of defects that form a *line* in the lattice structure.
- May arise during solidification (e.g. casting) or deformation (e.g. metal forming) processes
- Slip is the movement of dislocations through the lattice
- Useful for explaining mechanical behaviour:
  - Force for deformation much less than bond strength
  - Provides ductility
  - Control properties by blocking dislocation movement
- Two main types:
  - Edge DISLOCATIONS
  - Screw DISLOCATIONS



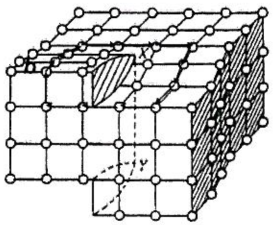
## Edge dislocation

- Edge dislocation
  - Extra plane of atoms $X'Y'YX$ in the regular lattice
  - Distorted and undistorted regions separated by line $XY$ (edge line)
  - Burgers vector $b$ gives the slip direction
    - Perpendicular to the edge direction



# Screw dislocation

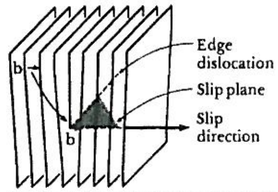
- Screw dislocation
  - Lattice structure is sheared by one spacing
  - Distorted and undistorted regions separated by line *XY* (screw line)
  - Produces a spiral in the lattice about the screw line
  - Burgers vector *b* gives the slip direction
    - Parallel to the screw line






# Slip planes and systems

- The Burgers direction and the dislocation line combine to form a slip plane
- The slip plane and direction give the *SLIP SYSTEM*
- Materials will deform preferentially along the slip planes
- Many slip systems possible in a single material




| Crystal Structure | Slip Plane | Slip Direction |
|---|---|---|
| BCC | {110}<br>{112}<br>{123} | ⟨111⟩ |
| FCC | {111} | ⟨110⟩ |
| HCP | {0001}<br>{11$\bar{2}$0}<br>{10$\bar{1}$0}<br>{10$\bar{1}$1} See note | ⟨100⟩<br>⟨110⟩ |

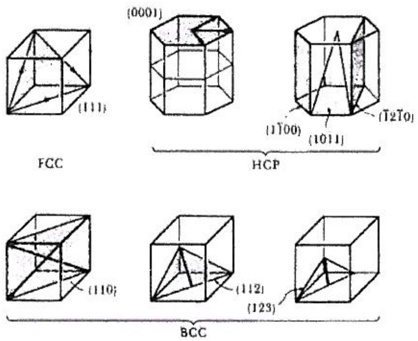
*Note:* These planes are active in some metals, alloys, or at elevated temperatures.



# Common slip planes in unit cells

Body-centred-cubic

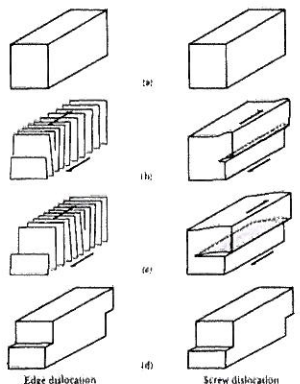
- BCC has up to 48 slip planes
- If slip planes intersect, a dislocation can change plane to avoid an obstruction
  - *"Cross Slip"*





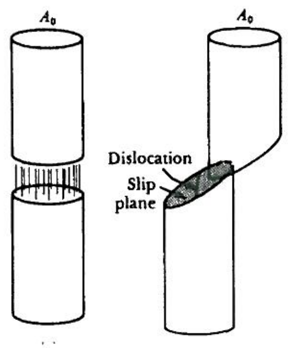

# Movement of dislocations

- Both edge dislocations and screw dislocations can move through the Crystal Lattice (slip)
- Deformation is the length of the Burgers vector



## Slip mechanism

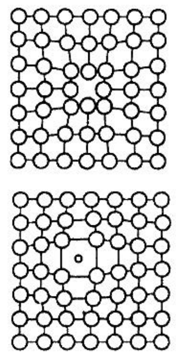
- Force required for slip is much less than for bond breakage
- Only bonds along the line defect need to be broken.
- Preventing slip increases material strength






## Point defects

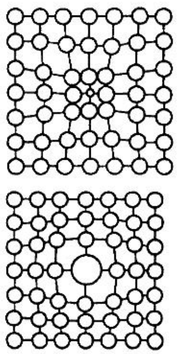
- Single atom defect in the lattice
- Prevents dislocation movement
- Vacancy
  - One atom is missing from the regular lattice
- Interstitial impurity
  - An extra atom occupies an abnormal position
  - Extra atom may be different from the rest of the lattice





## Substitutional point defects

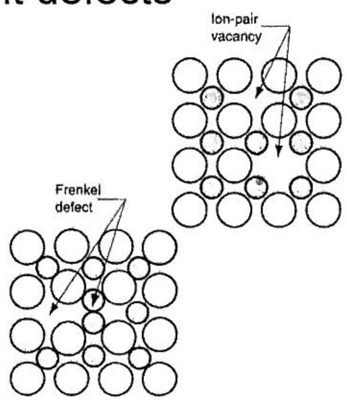
- An atom in the lattice is Replaced by an atom of a different element
- Usually present as alloying elements or impurities
  - Solid solution strengthening
- Relative size of substitutional atom deforms the regular lattice
  - Different material properties





## Ionic point defects

- Overall charge balance maintained in the material
- Schottky defect
  - Missing anion-cation pair
- Frenkel defect
  - Ion moved from regular lattice position to an Interstitial site



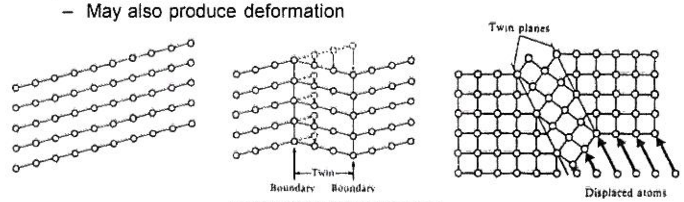
## Surface defects

- Surface defects are boundaries that separate regions having the same crystal structure but different orientations
  (NOT THE EXTERNAL SURFACE OF A MATERIAL)
- Three most common types:
  - Twin BOUNDARIES
  - Stacking FAULTS
  - Grain BOUNDARIES



## Twin boundaries

- Twin boundaries or *twin planes* exist where there is a mirror-image misorientation of the lattice
  - Always occur in pairs
  - interfere with slip
- Often caused by a shear force shifting the atoms out of position
  - May also produce deformation





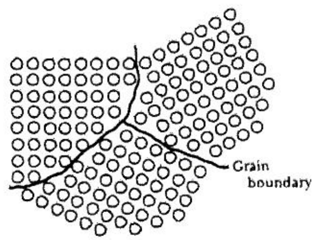

## Stacking faults

- Stacking faults are errors in the stacking sequence that occur in FCC metals
  - Perfect FCC lattice: *ABCABCABCABCABC……*
  - Missing *C* layer: *ABCABCABABCABCABC……*
- Small region with a HCP stacking sequence
- Stacking faults interfere with slip



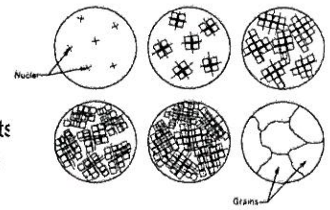
## Grain Boundaries

- A *grain* is a portion of a material within which the atomic arrangement is identical
- Orientation of the atomic arrangement is different for each adjoining grain
- Separated by *grain boundaries* where atoms are not properly spaced
  Too close – compressive region
  Too far apart – tensile region



## Polycrystalline Materials

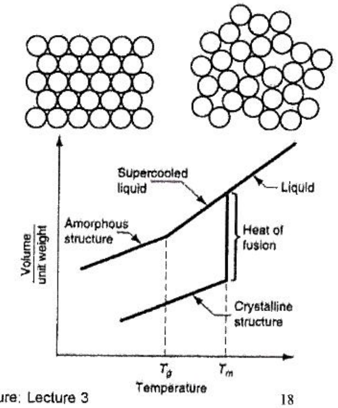
- Polycrystalline materials form from a large number of small Randomly orientated crystalline grains
- Grains form when a liquid material solidifies and crystallisation starts simultaneously at several points
- A small grain size means more grain boundaries
  - prevents slip
  - increases strength






## Non-Crystalline (Amorphous) Solids

- Crystalline materials exhibit long range order and a step change in volume
  Solid ⇔ Liquid @ $T_m$
- Amorphous materials exhibit short range order only and are less densely packed
  Solid @ $T_g$
- Glass, rubber and many polymers are amorphous
  - Also some metals at fast cooling rates



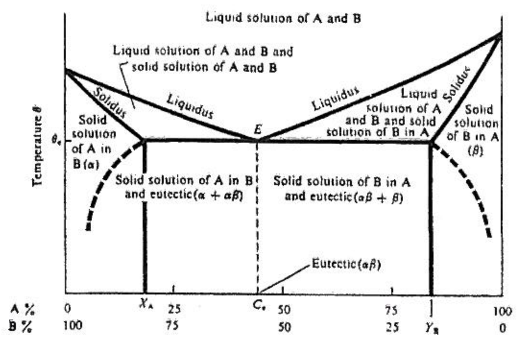



## Equilibrium phase diagrams

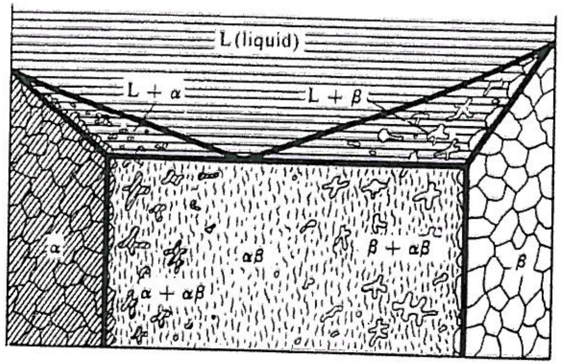
- Useful to predict critical temperatures and material phases present in an alloy or mixture of metallic and non-metallic elements
  - Cu-Ni, Fe-C
- *LIQUIDUS* – entirely liquid above this line
- *SOLIDUS* – entirely solid below this line
- *SOLVUS* – line denoting the limit of solid solubility of one phase in another
- Most solid solubility varies with temperature
  - Exploited in *solid solution strengthening*
- *EUTECTIC* - a specific composition ($C_E$) that has a unique freezing point, *E*
  - Single-phase liquid solidifies into a mixture of two solid phases ($L \rightarrow \alpha\ \beta$)
  - Lamellar arrangement of α and β called the *eutectic microconstituent*



## Phase diagram - partial solubility



## Physical state of various phases






## Other phase transitions

- *EUTECTOID* – a single-phase solid changes into a two-phase solid mixture (point *E'*)

  $(\gamma \rightarrow \alpha + \beta)$

- *PERITECTIC* – a two-phase solid-liquid mixture transforms into a single-phase solid

  $(L + \delta \rightarrow \gamma)$

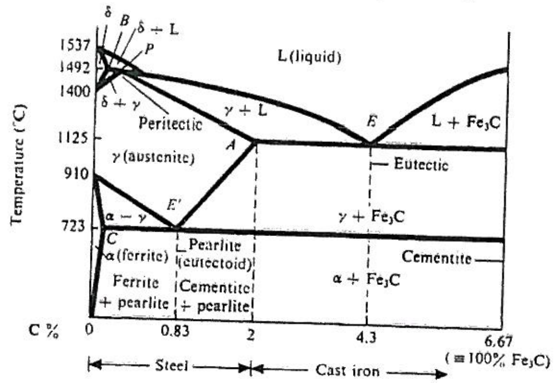
- *PERITECTOID* – a two- phase solid-solid mixture changes into a single-phase solid

  $\alpha + \beta \rightarrow \gamma$

- *HYPO/HYPER EUTECTIC/EUTECTOID*
  - A composition above/below the eutectic/eutectoid mixture
  - e.g.: hypereutectoid



## Iron-Carbon (Fe-C) diagram

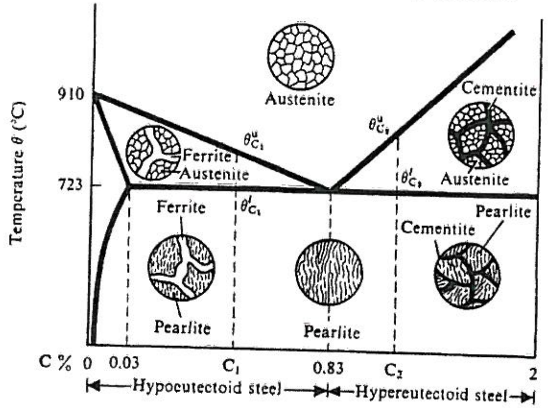





## Fe-C microstructures

- All the carbon is present as $Fe_3C$ which contains 6.67 % carbon
- A composition with <2% C is known as steel and may contain the following microstructures
  - *CEMENTITE*: very hard, thin needle-like structure of $Fe_3C$
  - *AUSTENITE*: evenly grained structure of FCC iron ($\gamma$ -iron) containing some $Fe_3C$ in solid solution
  - *FERRITE*: soft BCC iron ($\alpha$ -iron) containing some $Fe_3C$ in solid solution
- Other structures form depending on the rate of cooling
  - *PEARLITE*: lamellae of ferrite and cementite (eutectoid microstructure)
    - Formed during slow cooling
  - *MARTENSITE*: ferrite supersaturated with dissolved cementite, very hard and brittle

# Microstructures in steels



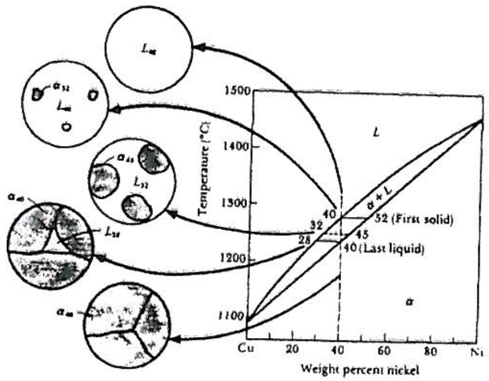



# Solidification

- When a molten alloy cools, its solidification depends on the cooling rate
- *Equilibrium solidification*
  - Slow enough to allow atoms to diffuse and produce a uniform structure
  - Usually impractical
- *Non-equilibrium solidification*
  - Occurs at rapid (practical) cooling rates
  - A non-uniform composition results where material is segregated into regions rich in one or other of the constituents
  - The average composition of the new solidified material produces a *non-equilibrium solidus* that diverges from the equilibrium solidus
  - In a eutectic system, once the eutectic composition is reached, all the remaining liquid solidifies

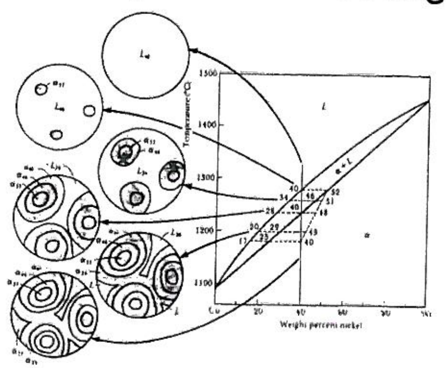


# Equilibrium cooling



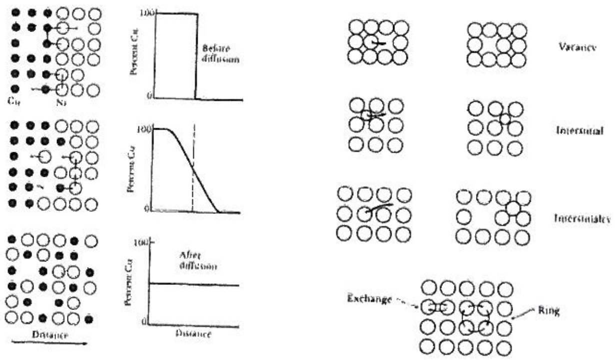



# Non-equilibrium cooling




The change in structure of a Cu-40% Ni alloy during nonequilibrium solidification. Insufficient time for diffusion in the solid produces a segregated structure

# Diffusion mechanisms






# Fick's 1st Law of mass diffusion

- Mass diffusion requires the transfer of atoms or molecules across a boundary between two materials in contact
  - Liquid-solid and solid-solid boundaries

$$\frac{dm}{dt} = -DA\frac{dc}{dx}$$

- $dm/dt$ is the rate of mass transfer
- $D$ is the diffusion coefficient of the material
  - Increases rapidly with temperature
- $A$ is the interface area
- $dc/dx$ is the Concentration gradient



# Inverse lever rule

- Used to determine relative amounts of each phase at a particular temperature and composition
  - Proportion of liquid phase (by mass)

$$L\% = \frac{CS}{LS}x100$$

  - Proportion of solid phase

$$S\% = \frac{LC}{LS}x100$$

  - Also applies to mixtures of solid phases