Materials: Metals and Alloys

PRRE1003

Resources, Processes & Materials Engineering

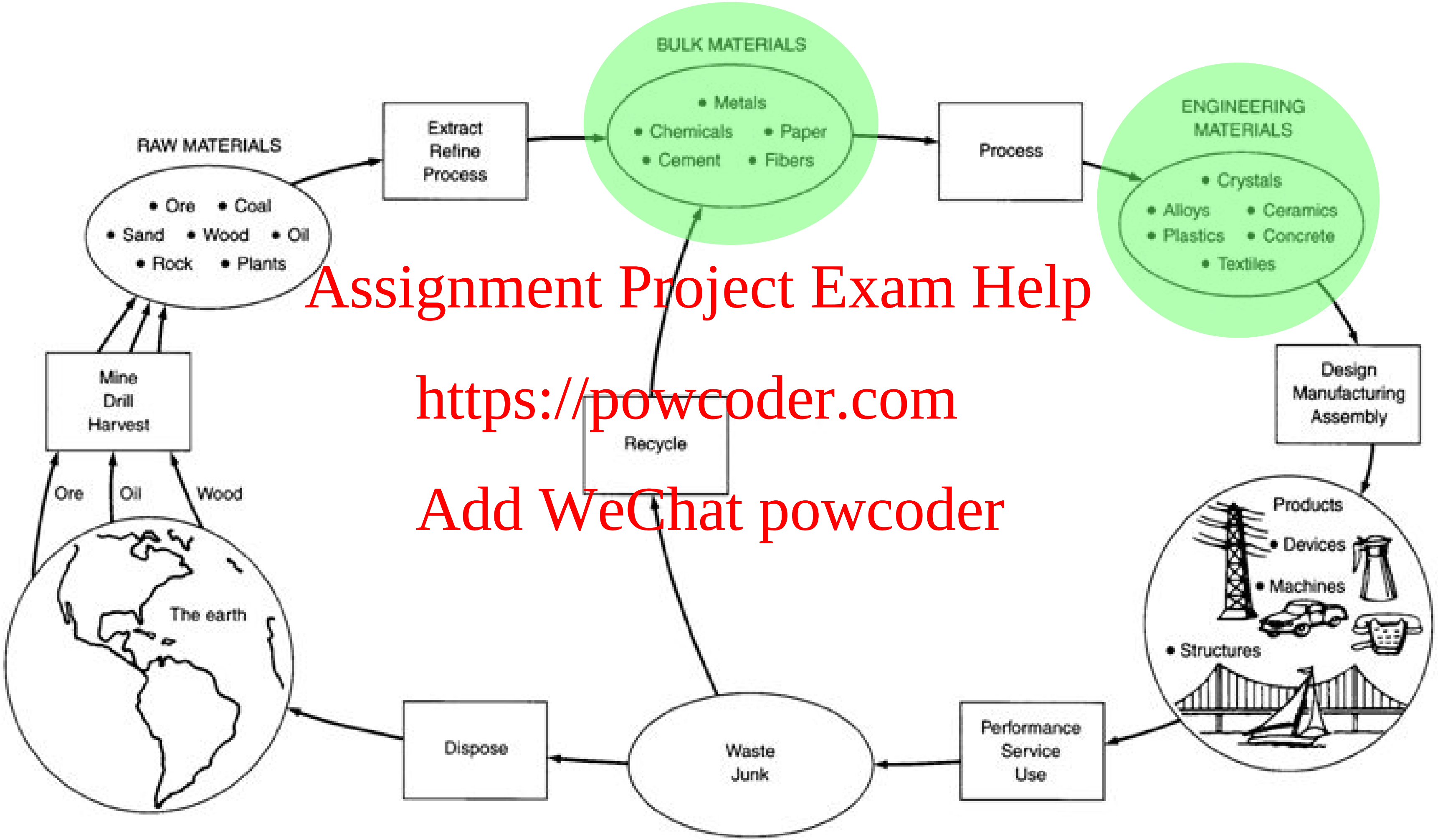
LECTURE M1

Dr Sofia Hazarabedian

maria.hazarabedian@postgrad.curtin.edu.au

Curtin University

Electronic Warning Notice



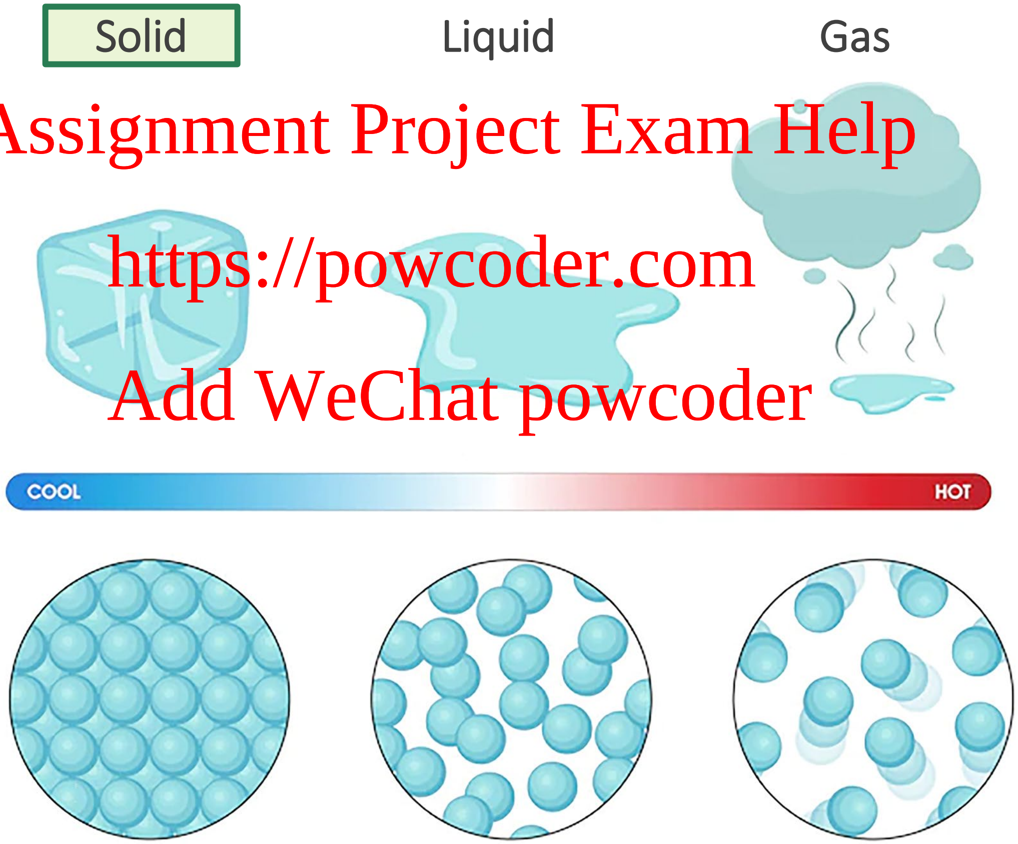
Reproduced from "Materials and Man's Needs", National Academy of Sciences, Washington D.C., 1974.

Lecture Outline

- What are 'raw' or 'bulk' materials?
- What are engineering materials? Do they matter? Are they matter?
- Gases, Liquids, **Solids**
- Focus on **Solids**
  - What holds them together? Bonding, structure, order, crystalline, amorphous.
  - Classifications – Metals, Polymers, Ceramics, Composites
- **Crystal Structures and Crystallography**
  - Simple Cubic, BCC, FCC, HCP and Miller Indices
  - Polycrystalline metals and crystal imperfections- vacancies and dislocations
- **Strengthening Mechanisms in Metallic Materials**
  - Elastic and Plastic Deformation - dislocations and slip systems
  - Mechanical properties in relation to structure
  - Crystal (grain) size, work hardening
  - Alloying

(Reference and extract sources in this section - *Materials: Engineering, Science, Processing and Design 3E;* M Ashby, H Shercliff, and D Cebon. [Ashby]
Materials Science and Engineering-An Introduction 10E; WD Callister and DG Rethwisch. [Callister])

Matter is commonly found on Earth in the following states



Material Bonding

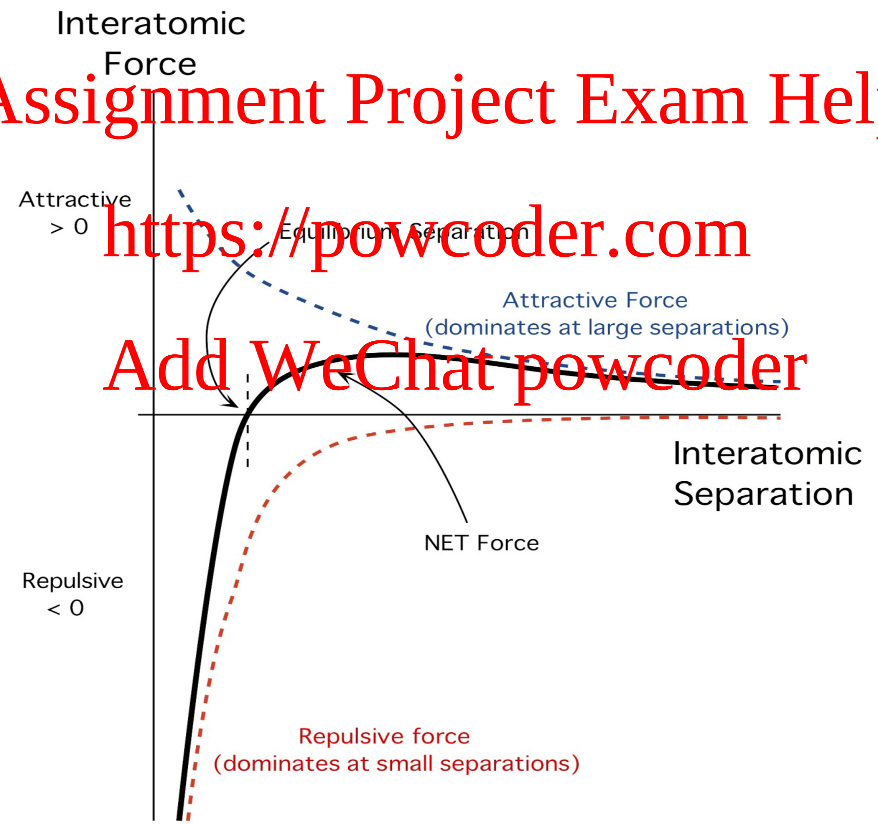
- As two atoms come close together they experience attractive forces between the (negative) electron clouds and the (positive) nuclei.

- The two atoms also experience the repulsive force between the two nuclei as well as the repulsive force between the two electron clouds.

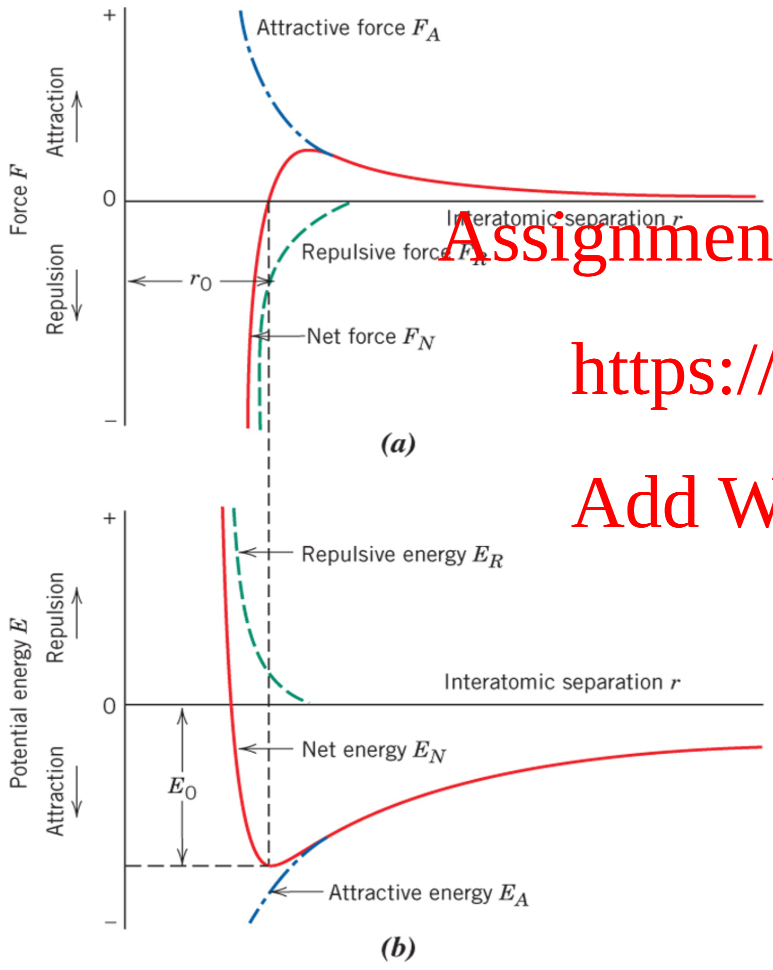
- At a separation (r_o) the sum of both the attractive forces and the repulsive forces equals zero.

- Significant other parameter - Temperature

Force against distance for approaching atoms



Force and energy in relation to interatomic spacing (Callister Pg. 30)



- Where there is no net force ($\sum F = 0$) or minimum net energy, a state of equilibrium exists and the centres of the two atoms will remain separated by the equilibrium spacing (r_0) or bond-length.

- The bonding energy (E_0) between two atoms corresponds to the energy at r_0, and represents the energy required to separate them.

Solid Material - Bonding

Types of interatomic and intermolecular bonds

- Primary (strongest bonds)
- Ionic
- Covalent
- Metallic

- Secondary (Weaker)
- Van der Waals
- Hydrogen

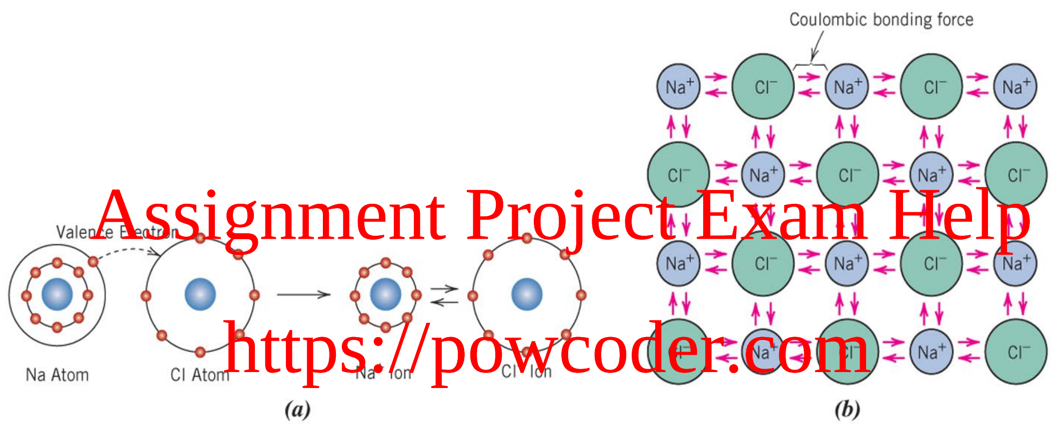
Substance	*Bonding Energy (kJ/mol)*	*Melting Temperature (°C)*
	Ionic	
NaCl	640	801
LiF	850	848
MgO	1000	2800
CaF_2	1548	1418
	Covalent	
Cl_2	121	−102
Si	450	1410
InSb	523	942
C (diamond)	713	>3550
SiC	1230	2830
	Metallic	
Hg	62	−39
Al	330	660
Ag	285	962
W	850	3414
	van der Waals[a]	
Ar	7.7	−189 (@ 69 kPa)
Kr	11.7	−158 (@ 73.2 kPa)
CH_4	18	−182
Cl_2	31	−101
	Hydrogen[a]	
HF	29	−83
NH_3	35	−78
H_2O	51	0

[a]Values for van der Waals and hydrogen bonds are energies *between* molecules or atoms (*inter*molecular), not between atoms within a molecule (*intra*molecular).

(Callister Pg. 34)

Primary Bonds

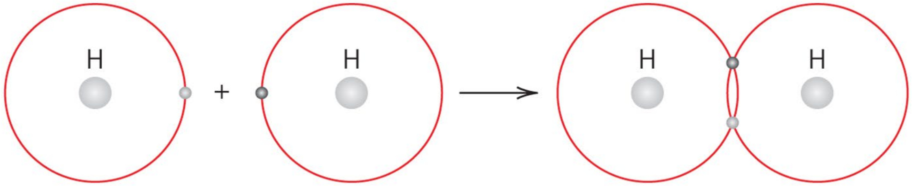
Ionic Bonding



(Callister Pg. 33)

- Found in compounds that are composed of both metallic and non-metallic ions; eg. Na^+Cl^-
- The attractive forces are Coulombic, i.e., positive and negative ions attract one another.
- Ionic bonding is non-directional, i.e. the magnitude of the bond is equal in all directions around an ion.
- Bonding energies between 600 – 1500 kJ/mol.
- Ionic-bonded materials have high melting points, hard, brittle, stiff, poor electrical and thermal conductors.

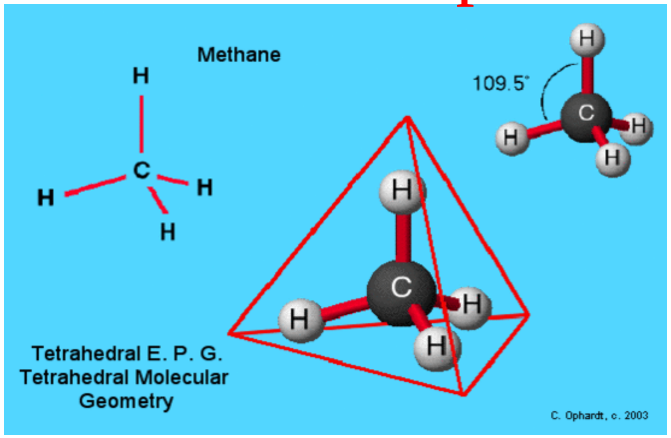
Covalent Bonding



•Covalent bonding involves the sharing of electrons between adjacent atoms.

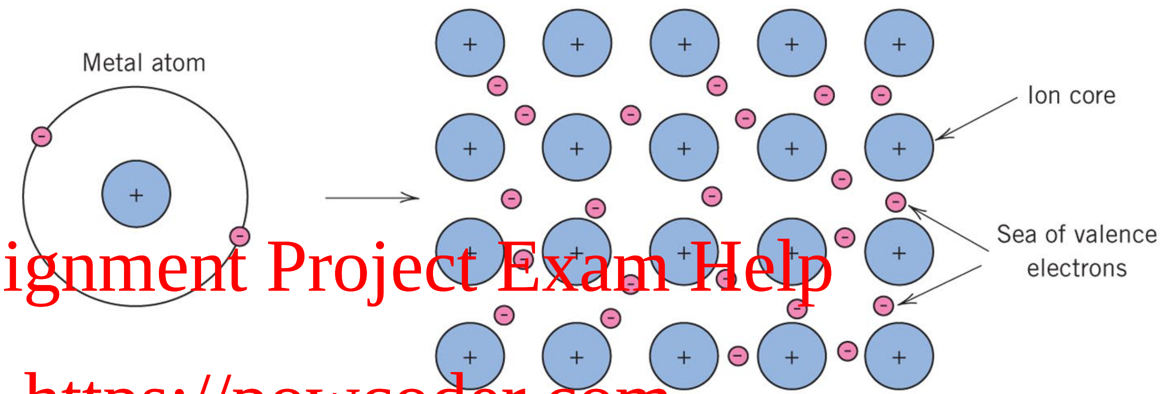
•Found in non-metallic molecules (H_2, Cl_2, F_2, H_2O, HF) and solids (Si, Ge, GaAs, SiC, diamond) as well as polymeric materials (e.g., plastics, rubbers).

•Covalent-bonded solids may be
- very strong, hard, stiff, brittle and high melting point (e.g., diamond)
- very weak with low melting point (e.g. Bismuth melts at 270°C).



Primary Bonds

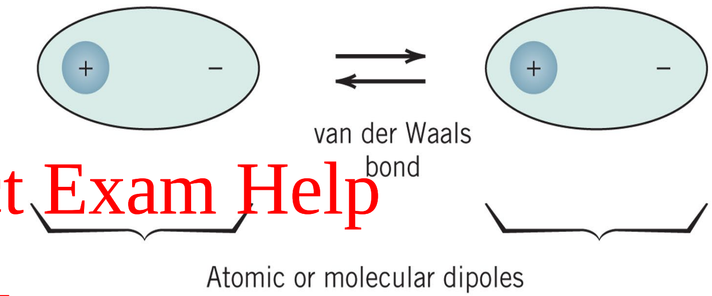
Metallic Bonding



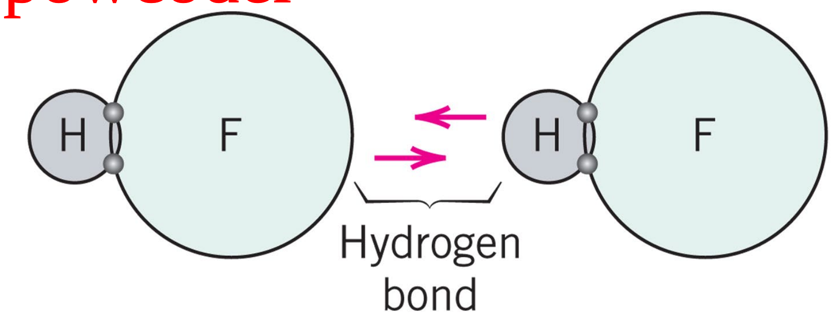
- Ions in a ‘sea ‘ of electrons
- Metallic bonding involves the attraction between ion cores and valence electrons
- Common in metals and their alloys
- The free valence electrons act as a “glue” to hold the ion cores together.
- Bonding may be weak with low melting point (e.g., Hg) or strong with high melting point (e.g., W).
- Presence of mobile electrons means good heat and electrical conductivity, and in terms of mechanical properties enables the feature of ductility in many metallic materials .

Secondary Bonds

Van der Waals and Hydrogen bonding



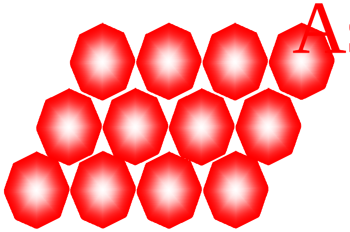
- Very weak when compared to the primary bonding.
- Bonding arises from attraction between atomic or molecular dipoles.

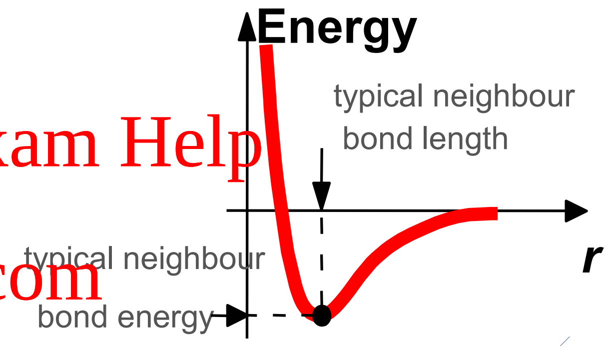


Structure and order

Crystalline and amorphous solids

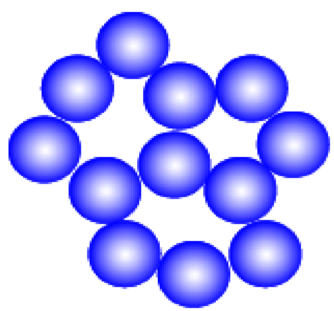
Crystalline • Dense, ordered packing

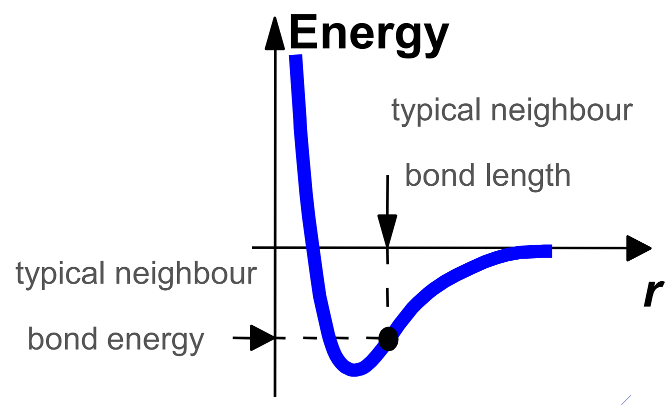




Dense, ordered packed structures tend to have lower energies.

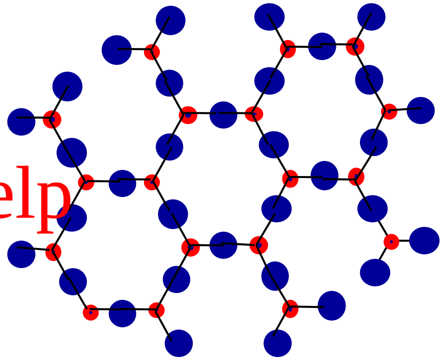
Amorphous • Non dense, random packing



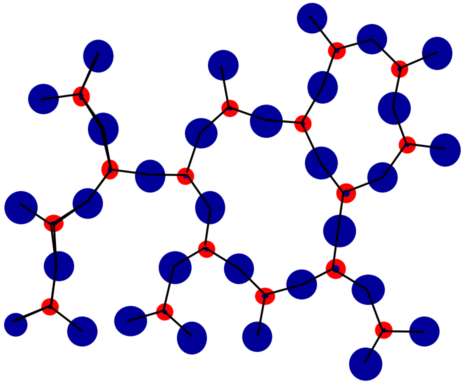


Crystalline and amorphous

- Crystalline materials – atoms pack in regular periodic 3D arrays
- Typical of
  - Metals
  - Many ceramics
  - Some polymers

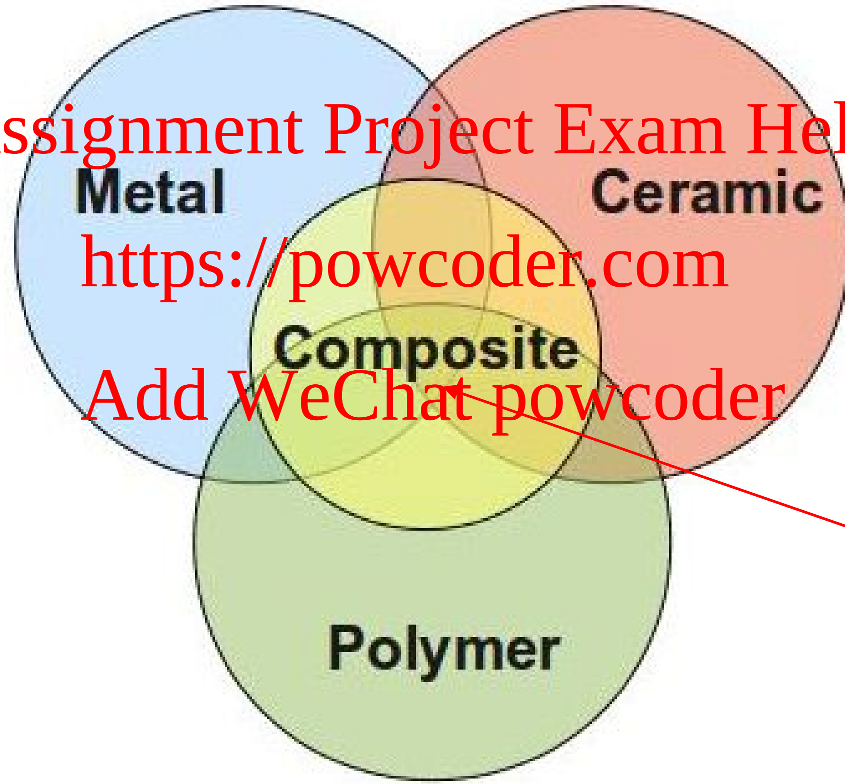


- Amorphous (Non –Crystalline) materials – atomic arrangement is purely random
- Typical of
  - Many polymers
  - Glasses
  - Complex structures
  - Rapidly solidified solids



Families of Materials

Steels, Aluminium, Nickel, etc.



Alumina, SiC, PS Zirconia, etc.

GFRP, CFRP, Concrete, Wood, etc.

Polyethylene, Teflon, Rubber, etc.

....focus on Metals.....

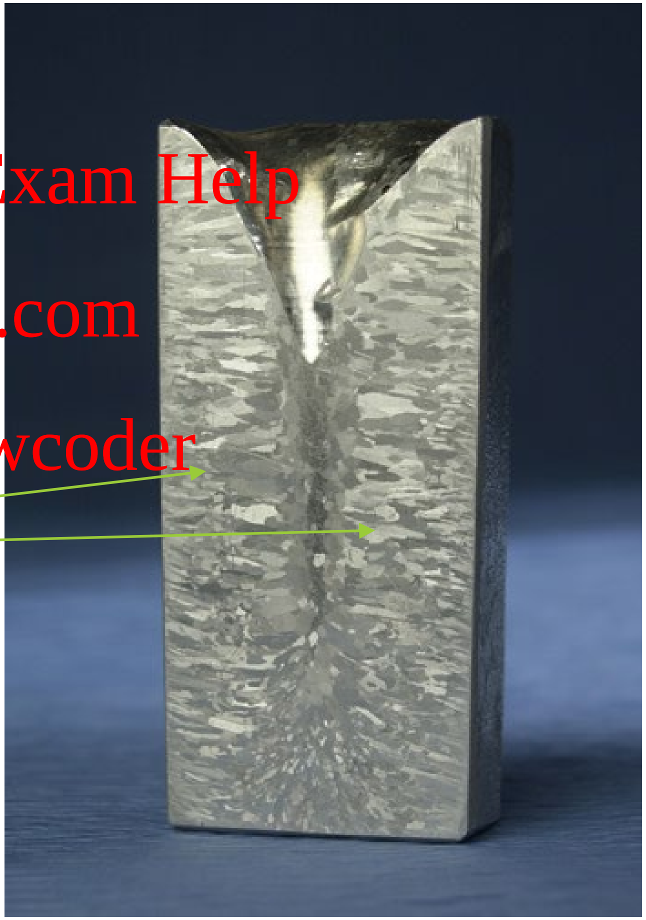
Learning Outcome Check 1

- Explain the following terms and give an example of each:
  - *metal*
  - *alloy*
  - *glass*
  - *ceramic*
  - *polymer*
  - *composite*

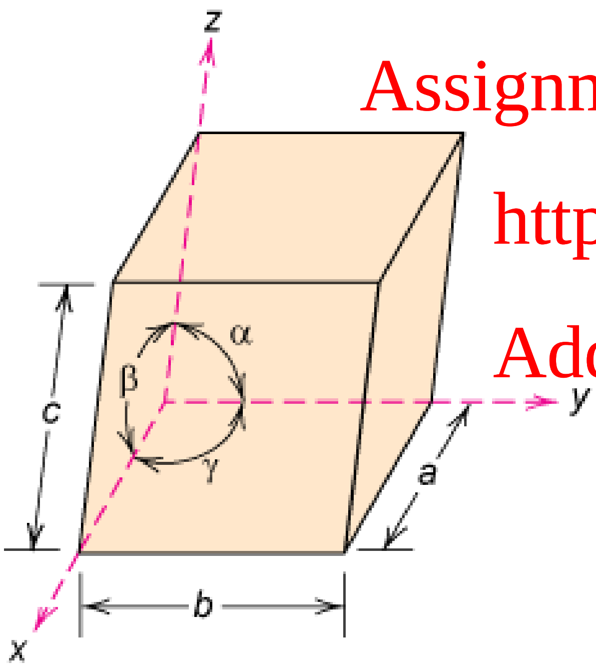
- Which type of bonding is predominant in each type of material above?
- What is the difference between a crystalline and amorphous structure?

Crystals and Grains in Metallic Materials

- The adjacent figure shows a section through an ingot of cast aluminium.
- This has been obtained after the aluminium has been extracted from its ore, refined at high temperature in the molten condition and then allowed to solidify.
- In everyday life metallic materials generally appear as shiny, machined or perhaps painted or coated surfaces.
- However, deeper analysis shows that the bulk solid material consists of crystals, or grains.
- How and where the crystals form on solidification has a major bearing on the properties of these materials, and thus their applications.
- The crystal and grain structures need to be understood so that they can be modified to develop the useful engineering materials we have today and for the future.



Unit cell: smallest repetitive volume which contains the complete lattice pattern of a crystal.



Callister (Pg.59).

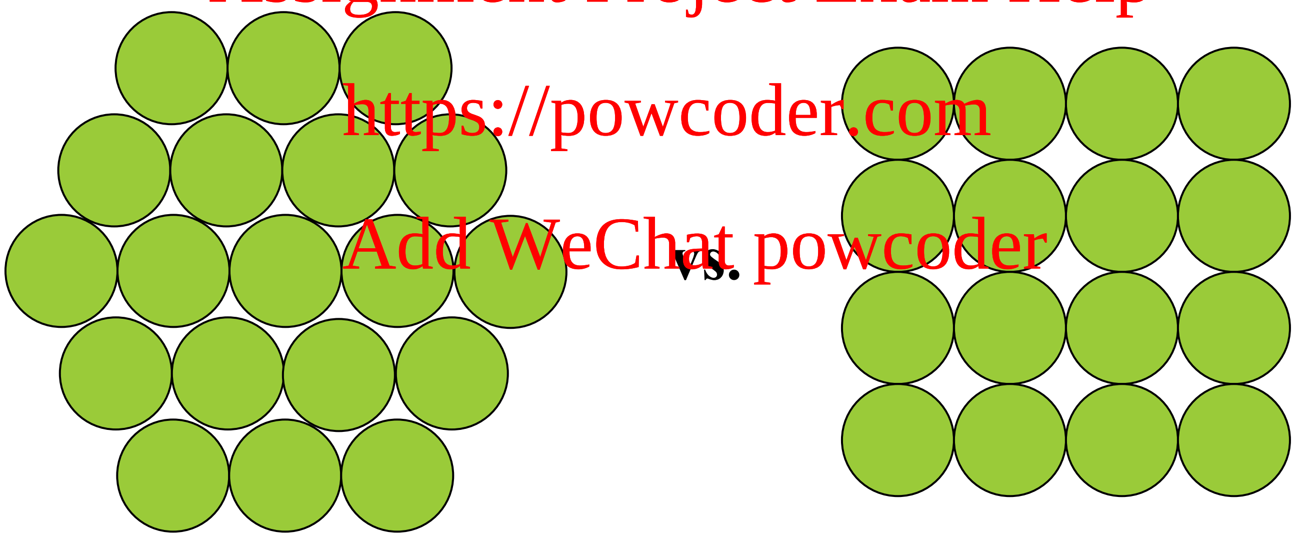
7 crystal systems

14 crystal lattices

a, *b*, and *c* are the lattice constants

How can we stack metal atoms to minimize empty space?

2-dimensions

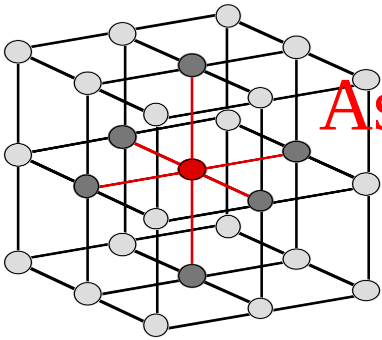


Now stack these 2-D layers to make 3-D structures

Crystal Structures and Crystallography (Ashby GL1-13)

Metallic Crystal Structures

- Simple Cubic **(SC)**



Reasons for metals' dense packing:

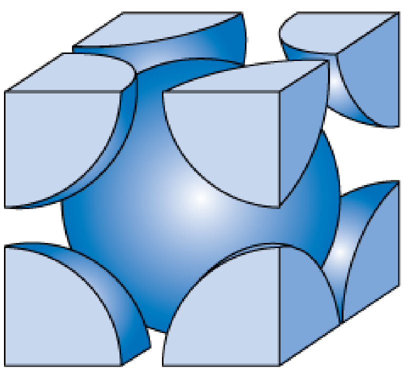
- Typically, only one element is present, so all atomic radii are the same.
- Metallic bonding is not directional.
- Nearest neighbor distances tend to be small in order to lower bond energy.
- Electron cloud shields cores from each other

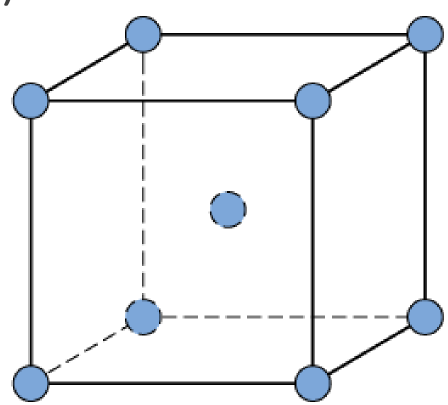
- Have the simplest crystal structures.

Coordination Number (CN) = Number of nearest neighbours

Atomic Packing Factor (APF) = $\frac{\text{Volume of atoms in unit cell}}{\text{Volume of unit cell}}$

- Body Centred Cubic **(BCC)**



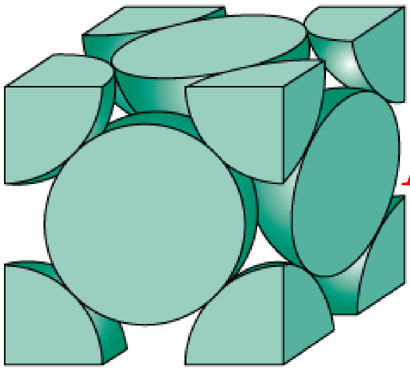


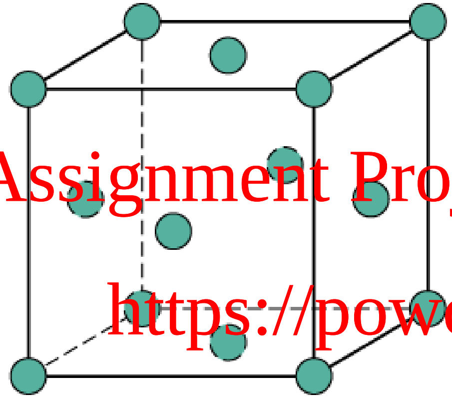
Examples:

- Iron
- Chromium
- Manganese
- Molybdenum

Metallic Crystal Structures

- Face Centred Cubic **(FCC)**

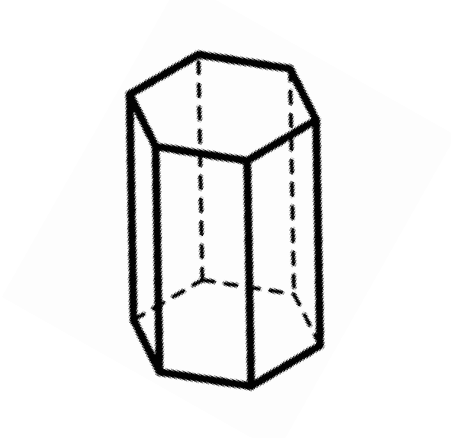


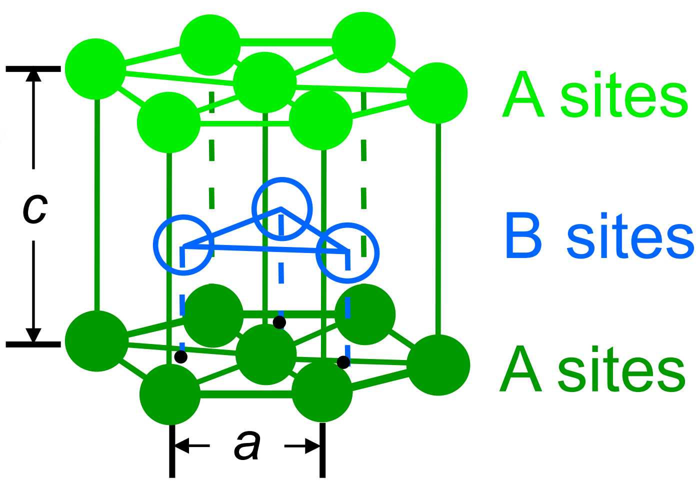


Examples:

- Nickel
- Gold
- Copper
- Aluminium

- Hexagonal Close Packed **(HCP)**





Examples:

- Titanium,
- Magnesium
- Zinc
- Zirconium

Miller Indices

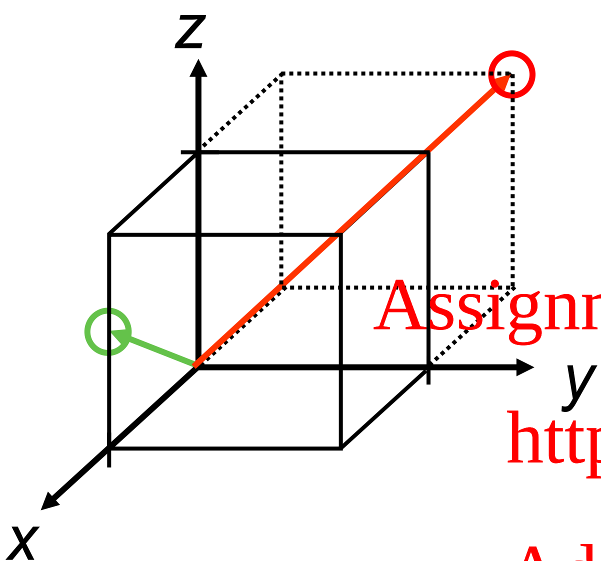
A pseudo-quantitative method of describing crystallographic orientations, i.e., atomic locations in terms of coordination, planes and directions.

Reciprocals of the (three) axial intercepts for a plane, cleared of fractions and common multiples.

All parallel planes have same Miller indices.

Principle

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)



Principle

1. Vector repositioned (if necessary) to pass through origin.
2. Read off projections in terms of unit cell dimensions *a*, *b*, and *c*
3. Adjust to smallest integer values
4. Enclose in square brackets, no commas [*uvw*]

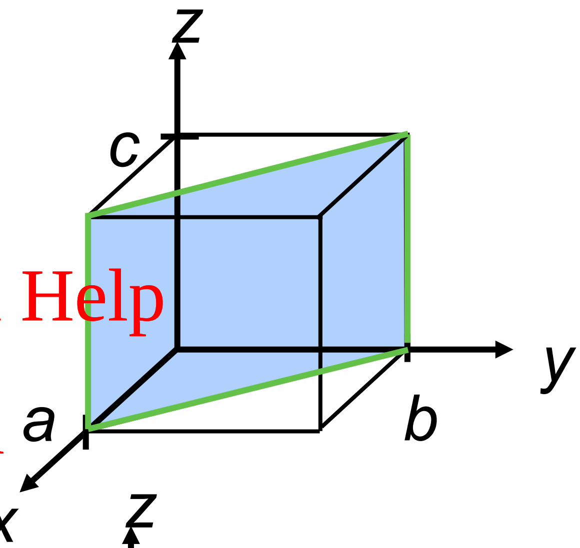
e.g. 1, 0, ½ => 2, 0, 1 => [201]

-1, 1, 1 => [$\bar{1}$11] where overbar represents a negative index

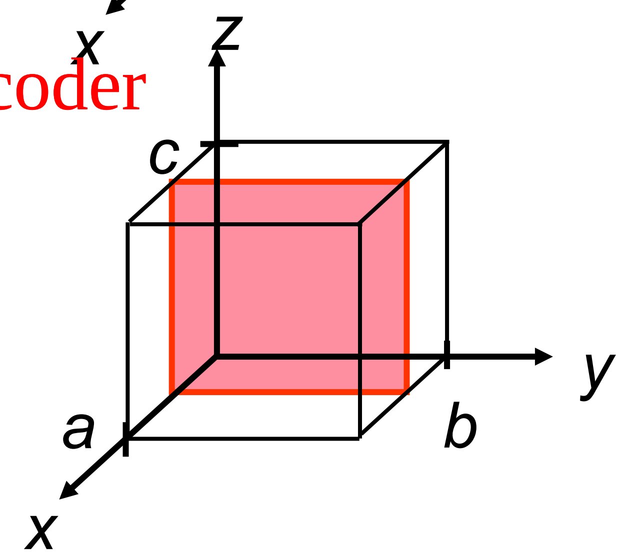
Families of directions represented by <*uvw*>

Crystallographic Planes

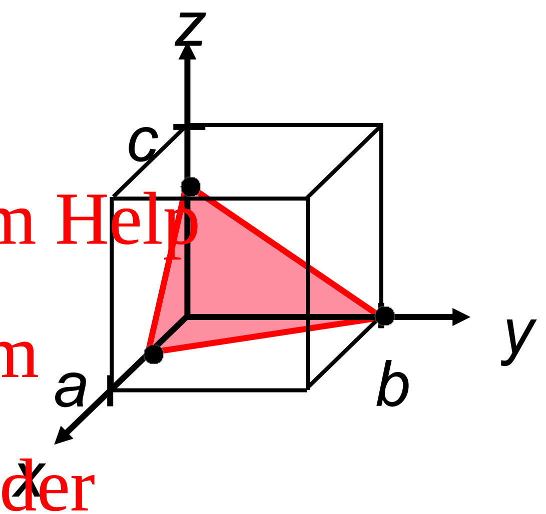
		a	b	c
1.	Intercepts	1	1	∞
2.	Reciprocals	1/1	1/1	1/∞
		1	1	0
3.	Reduction	1	1	0
4.	Miller Indices	(110)		



		a	b	c
1.	Intercepts	1/2	∞	∞
2.	Reciprocals	1/½	1/∞	1/∞
		2	0	0
3.	Reduction	1	0	0
4.	Miller Indices	(100)		



example		a	b	c
1.	Intercepts	1/2	1	3/4
2.	Reciprocals	1/½	1/1	1/¾
		2	1	4/3
3.	Reduction	6	3	4
4.	Miller Indices	(634)		



Family of Planes represented by $\{hkl\}$

E.g. $\{100\} = (100),(010),(001),(\bar{1}00),(0\bar{1}0),(00\bar{1})$

Densities of Material Classes (Callister)

In general

$\rho_{metals} > \rho_{ceramics} > \rho_{polymers}$

Why?

Metals have...

- close-packing (metallic bonding)
- often large atomic masses

Ceramics have...

- less dense packing
- often lighter elements

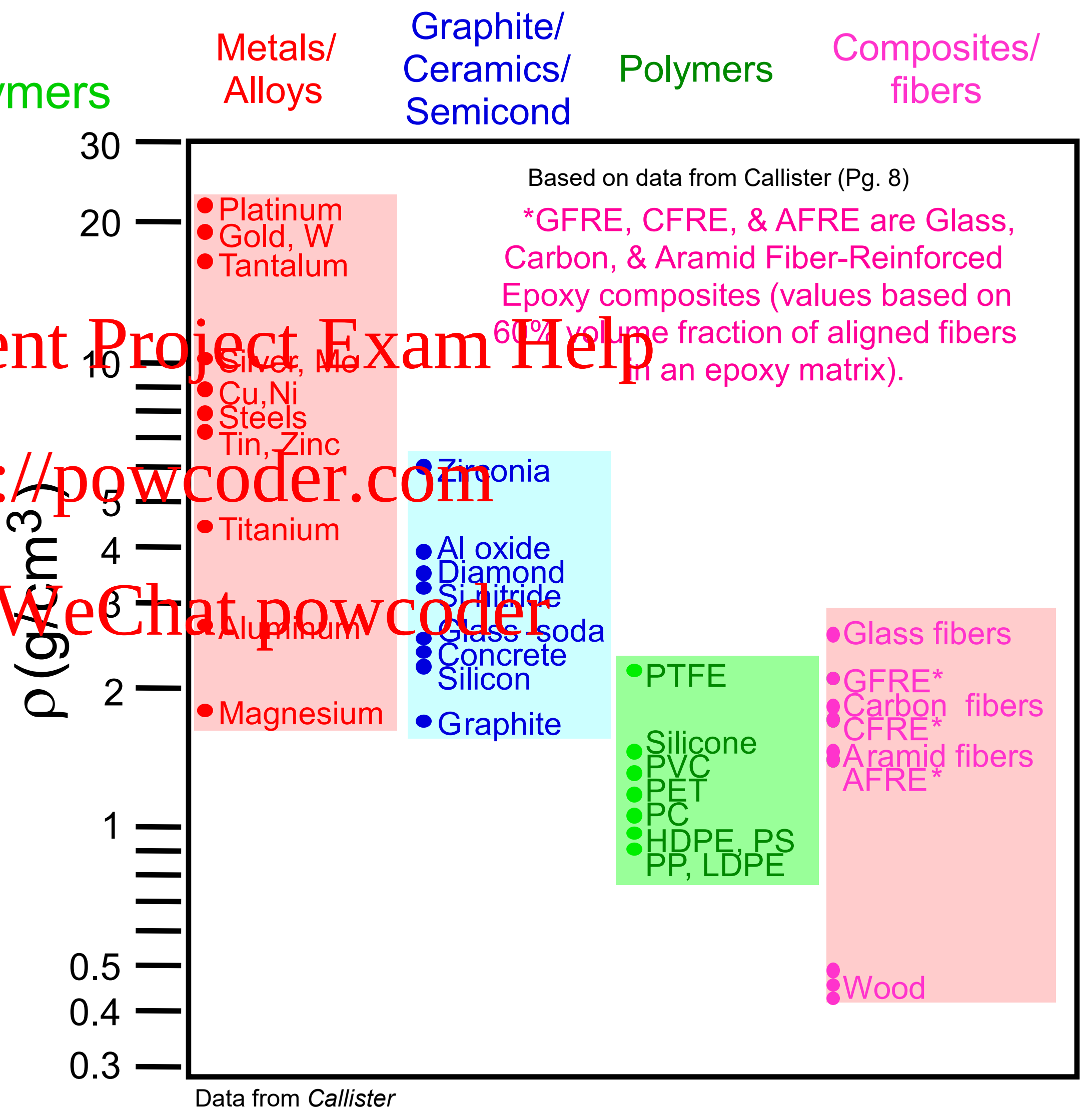
Polymers have...

- low packing density (often amorphous)
- lighter elements (C,H,O)

Composites have...

- intermediate values

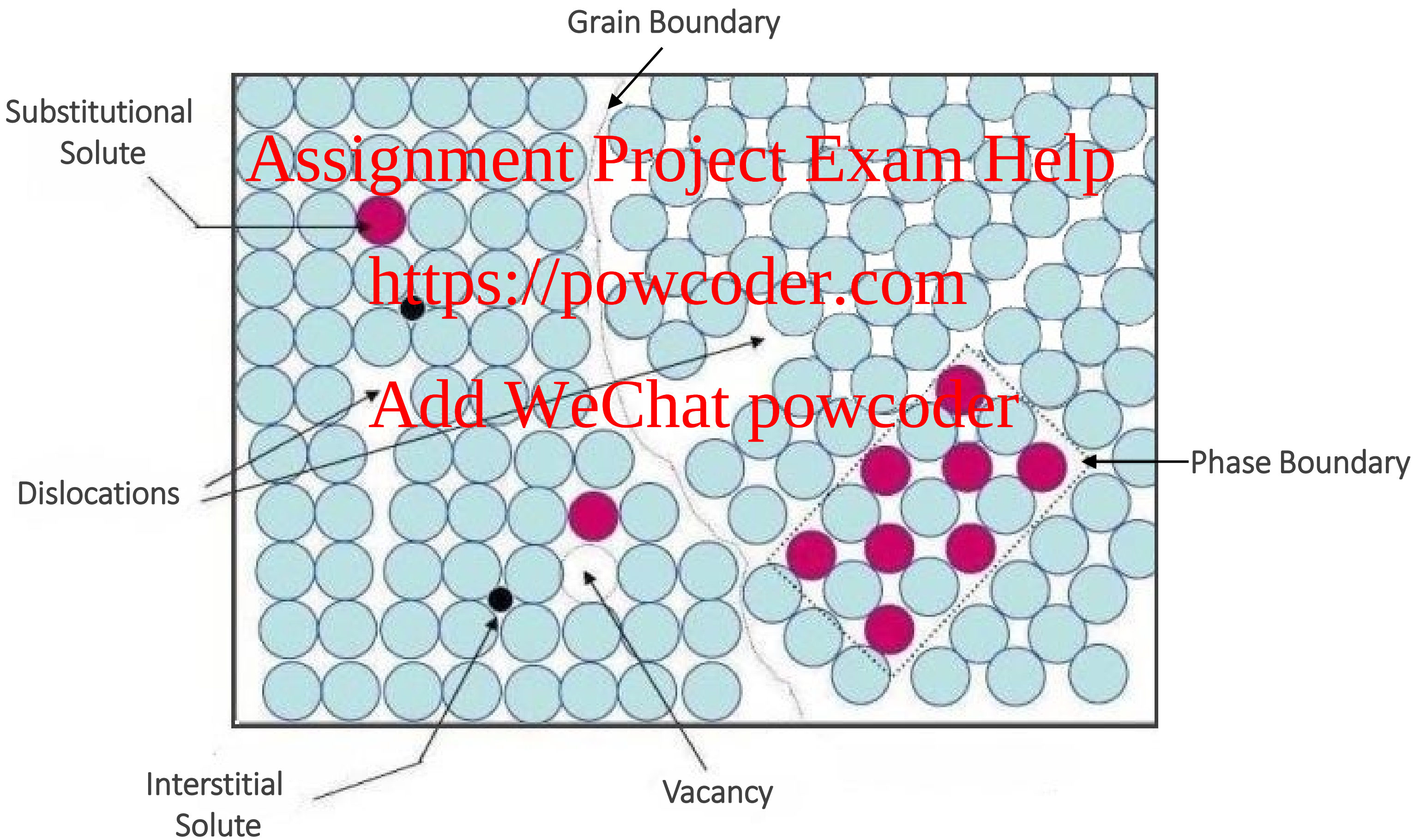
ρ: Density



Data from *Callister*

Imperfections and Defects in Crystals

Crystal Defects



Dislocations

Edge Dislocation

The edge of an extra portion of a plane of atoms, or a half-plane, terminates within the crystal

It is a linear defect, that centers on the line defined along the end of the extra half-plane of atoms (the dislocation line)

Screw Dislocation

Formed by a shear stress that is applied to produce the distortion shown in the Figure

The atomic distortion is also linear and along the dislocation line

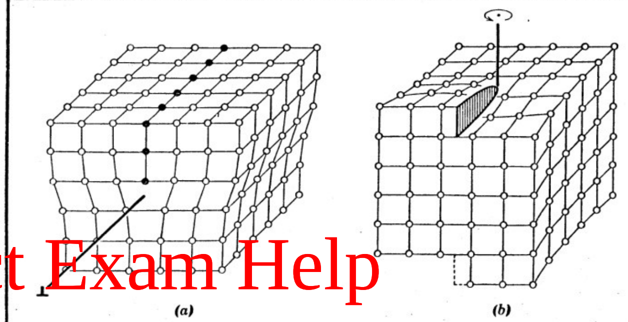


Figure 1 Geometry of simple dislocations. (a) Edge dislocation and (b) screw dislocation. The lines normally used to represent the dislocations are also indicated, as are the symbols for them, ⊥ and ⟲.

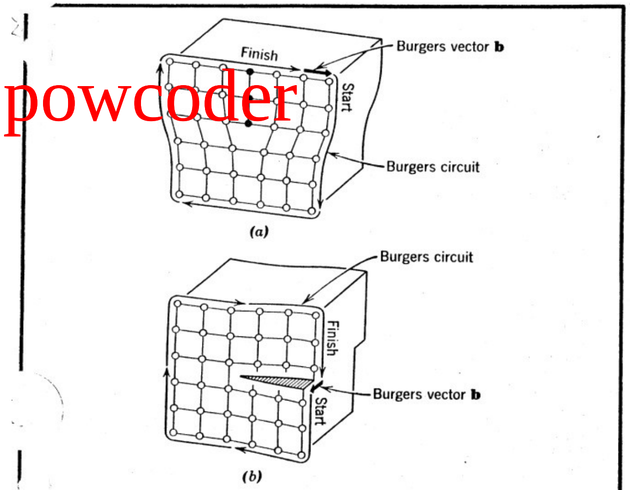


Figure 2 Burgers vectors and Burgers circuits of (a) an edge dislocation and (b) a screw dislocation.

Imperfections and Defects in Crystals

Dislocations

A transmission electron microscopy (TEM) image of a titanium alloy in which the dark lines are dislocations.
(Callister Pg. 105)

Learning Outcome Check 2

- What are Millers Indices used to represent?
- What is the difference between FCC, BCC and HCP crystal structures?
- Name three types of crystalline defects
- What are the two main types of dislocation

Strengthening Mechanisms in Metallic Materials (Ashby Pg. 128-163)

Elastic and Plastic Deformation

Fundamental Mechanical Properties

- **Strength**

  Usually considered as the tensile strength, which is defined as the maximum force required to fracture per unit cross sectional area in tension. In most cases however, the yield strength, the force at which the material begins to permanently deform, is the limiting factor

- **Ductility**

  This is considered to be the capacity to undergo deformation (generally under tension) without rupture. This is distinct from malleability

- **Toughness**

  This is the ability to withstand bending or deflection, or absorb energy, without fracture. Effectively, it is the resistance to fracture.

- **Hardness**

  This is ability to resist plastic deformation, indentation or abrasion. This property is very important in an engineering application where resistance to wear is a requirement.

Elastic Deformation

A result of an extension of the interatomic bonds, retractable after the load is removed (reversible)

It occurs when a material is loaded within its elastic limit and stress and strain are proportional

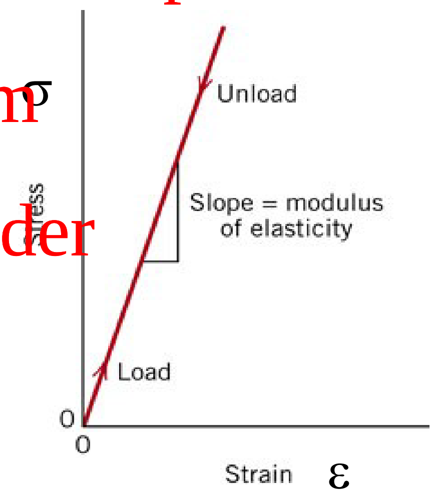
Hooke's Law:

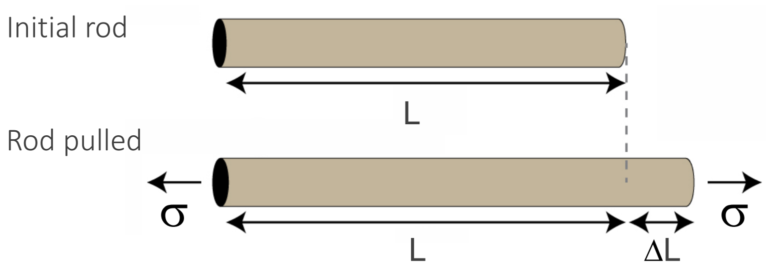
$$\sigma = E\,\varepsilon$$

σ: Stress [MPa]
E: Young's modulus or modulus of elasticity [GPa]
ε: Strain (no units)
F: Force [N]
A: Cross-sectional area [m^2]
L: Length [cm]

Where σ and ε are defined as:

$$\sigma = \frac{F}{A} \qquad \varepsilon = \frac{\Delta L}{L}$$

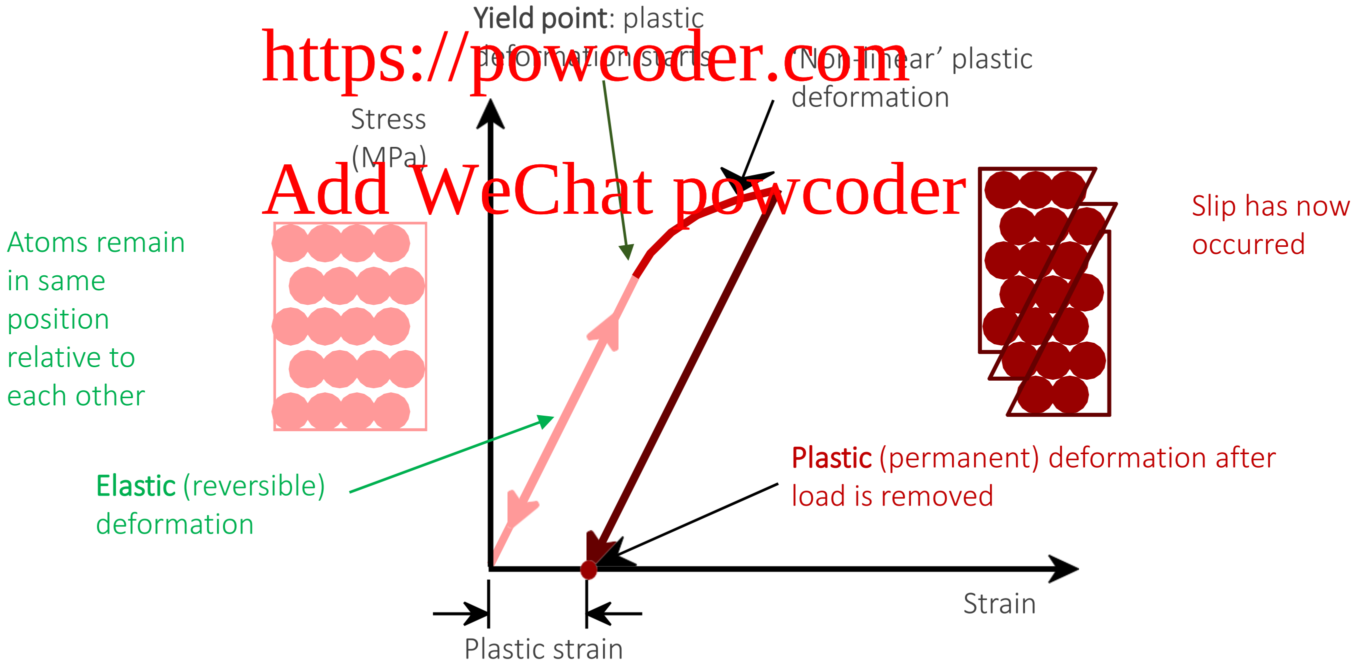




Plastic Deformation

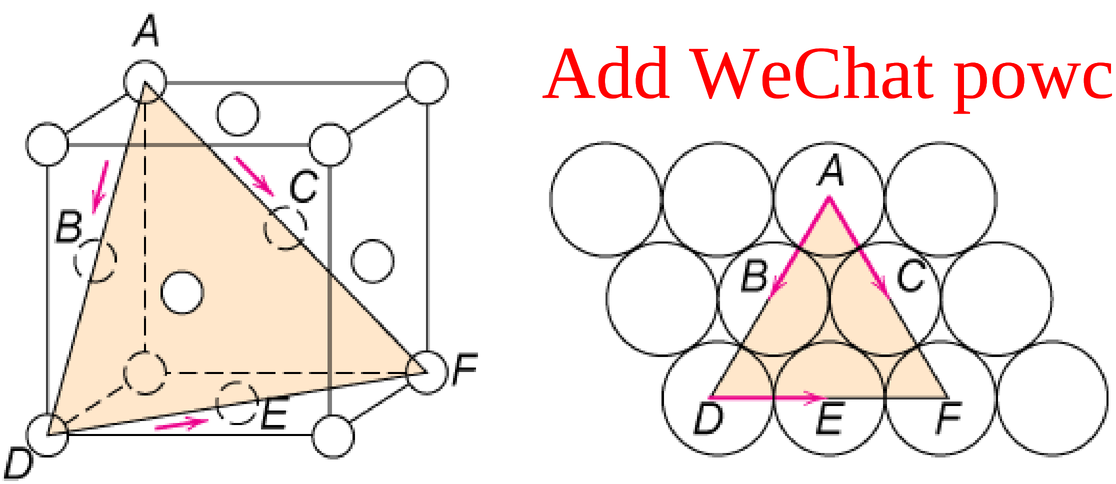
A result of interatomic bonds being broken and atoms moving to different positions relative to each other (irreversible or permanent deformation). This occurs when the material is loaded beyond its elastic limit.

Simple Tensile Test curve



Slip Systems and Dislocation Theory

- In crystalline solids, the plastic deformation process is also known as SLIP, as planes of atoms tend to slide over each other into new stable positions
- Slip occurs on close packed planes and in close packed directions within the crystal – so that the atoms can follow the shortest path to their new positions under the most favourable energetic conditions
- The combination of slip plane and slip direction is known as a *slip system*.



(a) (b)

Slip plane - plane on which easiest slippage occurs - highest planar densities (and large interplanar spacing)

Slip direction - directions of movement - highest linear densities

12 x {111}(110) systems in a FCC unit cell

(Callister Pg. 185)

Slip Systems and Dislocation Theory

Table 7.1 Slip Systems for Face-Centered Cubic, Body-Centered Cubic, and Hexagonal Close-Packed Metals

Metals	*Slip Plane*	*Slip Direction*	*Number of Slip Systems*
	Face-Centered Cubic		
Cu, Al, Ni, Ag, Au	$\{111\}$	$\langle 1\bar{1}0 \rangle$	12
	Body-Centered Cubic		
α-Fe, W, Mo	$\{110\}$	$\langle \bar{1}11 \rangle$	12
α-Fe,W	$\{211\}$	$\langle \bar{1}11 \rangle$	12
α-Fe, K	$\{321\}$	$\langle \bar{1}11 \rangle$	24
	Hexagonal Close-Packed		
Cd, Zn, Mg, Ti, Be	$\{0001\}$	$\langle 11\bar{2}0 \rangle$	3
Ti, Mg, Zr	$\{10\bar{1}0\}$	$\langle 11\bar{2}0 \rangle$	3
Ti, Mg	$\{10\bar{1}1\}$	$\langle 11\bar{2}0 \rangle$	6

(Callister Pg.186)

Dislocation Movement

- When slip occurs in crystals it has been shown that the energy measured to produce the deformation is approximately **1000 times** <u>less</u> than that expected by theoretical calculation.

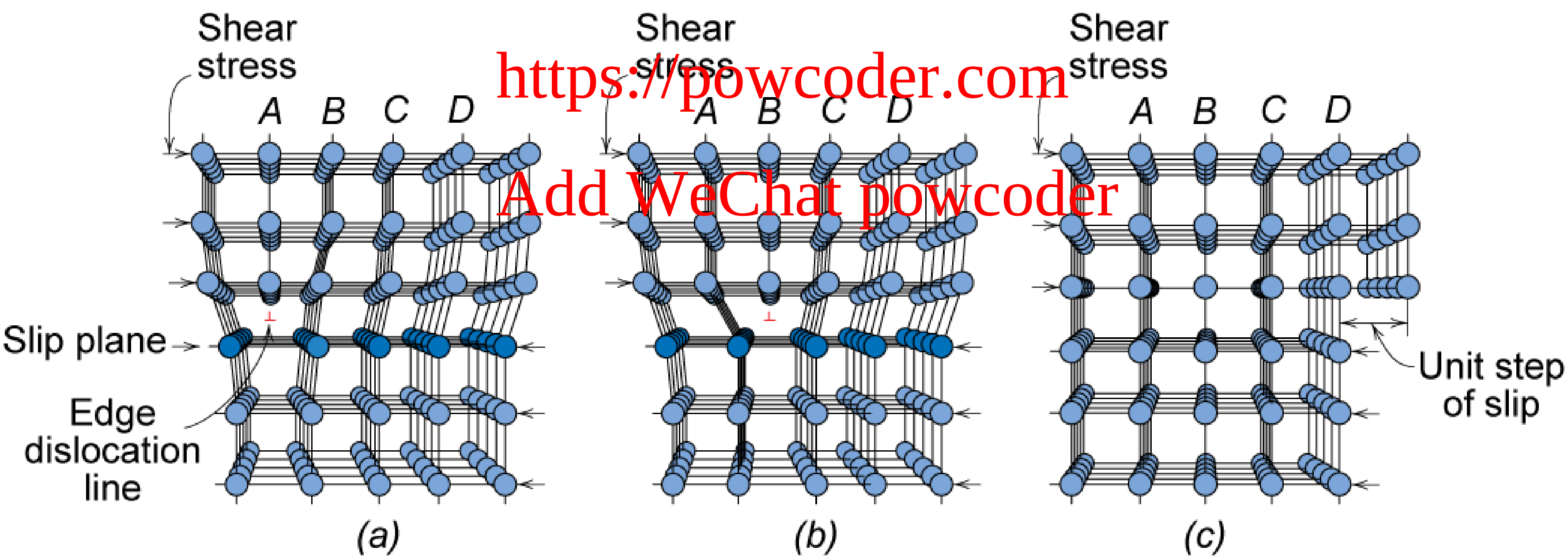
- Reason for discrepancy: theory assumes a perfect crystal structure and all atoms on slip plane move simultaneously.

- In practice, slip occurs by incremental movement of discrete slip events or half planes i.e., dislocations, which are also known as line defects or lines of (potential) energy

- In simple terms, it is the movement of these dislocations, individually or in combination, that produces slip in crystals, and therefore, permanent deformation in metals and alloys (and some ceramics).

Dislocation Movement

In metal crystals, an edge dislocation slides over adjacent plane half-planes of atoms.
If dislocations can't move, plastic deformation doesn't occur!



(Callister Pg. 183)

Strengthening Mechanisms in Metallic Materials

Dislocation Movement and Interaction

- During yield there is multiple dislocation movement, which eventually leads to interaction and entanglement of these lines. Entanglement restricts their movements. This restriction and therefore resistance to further deformation is known as work hardening or strain hardening.

- Any process or treatment that will restrict or prevent the movement of dislocations within the crystals or grains will result in strengthening (and hardening).

- **Strength is increased by making dislocation motion difficult.**

- Strength of metals may be increased by:
  - decreasing grain size
  - solid solution strengthening
  - precipitate hardening
  - cold working

Learning Outcome Check 3

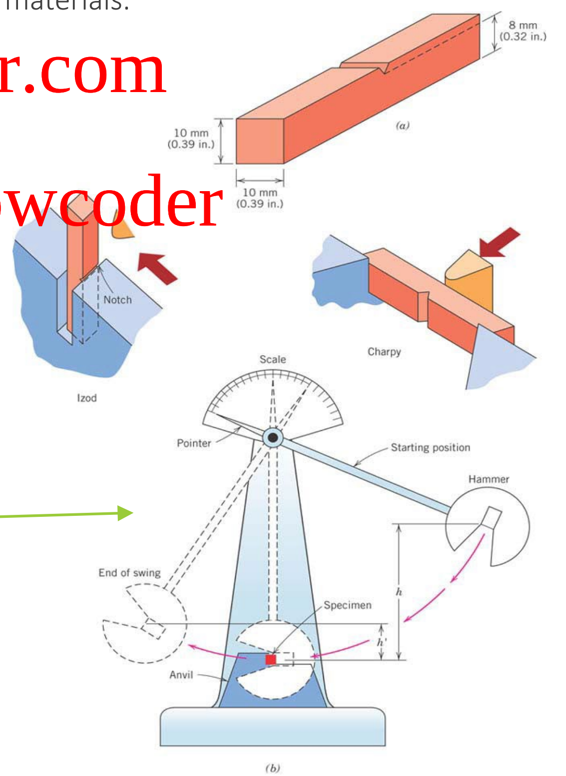
- What is the difference between strength and toughness?
- What is the overall principle behind strengthening metals?

Mechanical Properties in relation to Structure

How to define or determine these properties?... By testing...

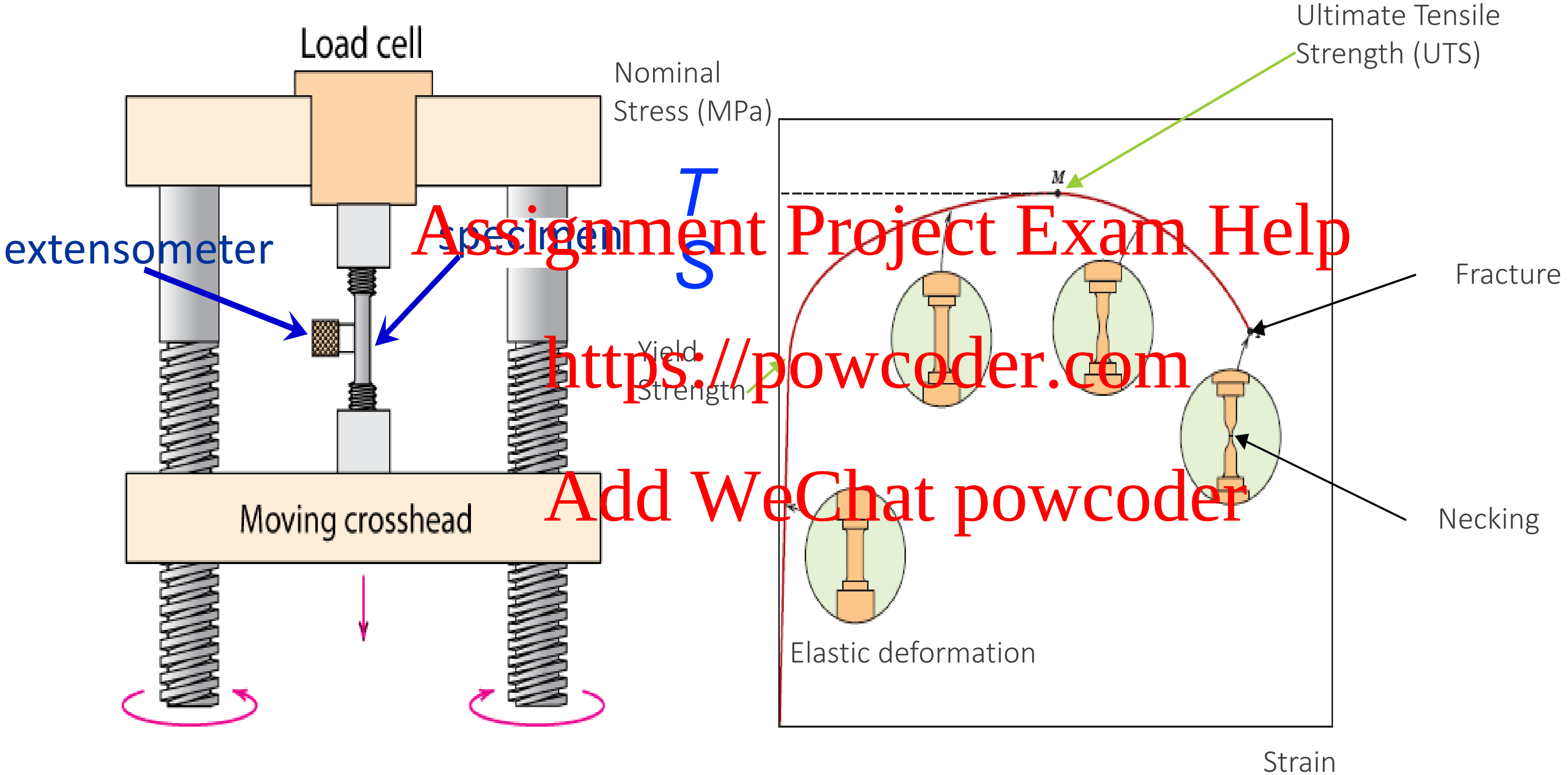
Primary Tests

- Tensile Test
  - One of the most valuable and commonly used of the mechanical tests for materials.
  - Data on strength, toughness and ductility
  - Expensive, relatively slow (loading rate) and destructive
  - Load capacity: a great range available
  - Loading method: mechanically or hydraulically
- Hardness Test
  - Surface indentation with a known load
  - Quick, low cost, semi destructive
- Impact Test
  - Strike standard specimen with calibrated pendulum load
  - Quick, intermediate cost, destructive



(Callister Pg.226)

Tensile Testing



Adapted from Fig. 6.3, *Callister & Rethwisch 8e.* (Fig.
6.3 is taken from H.W. Hayden, W.G. Moffatt, and J. Wulff, *The Structure and Properties of Materials*, Vol. III, *Mechanical Behavior*, p. 2, John Wiley and Sons, New York, 1965.)

Pure Metals

Copper (Electrical)

Aluminium (Electrical/Decorative)

Refractories (Mo, W) – High temperature

Nickel (Electrical, Electronic)

- Pure metals for load bearing applications are of little use.
- In order to improve mechanical properties (and many other properties) various mechanisms or treatments are employed, and **alloying** with other elements is performed.
- Alloying is either to neutralise the effect of undesirable trace elements, or to modify and improve desired properties for specific applications.

Strengthening Mechanisms in Metallic Materials

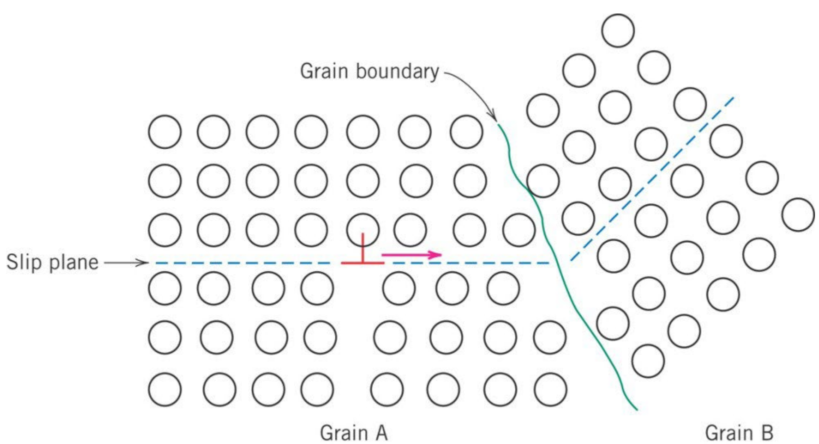
Strengthening by Reducing Grain Size

- Most commercial metals are made up of polycrystalline grains, of random crystallographic orientations, with a common grain boundary
- When these metals are subjected to loading, the dislocation motion must take place across the common boundary, from grain A to grain B
- The grain boundary acts as a barrier for dislocation, because:
  - the two grains are randomly orientated, a dislocation passing into B needs to change its direction of motion, which becomes more difficult as the misorientation increases
  - The atomic disorder within a grain boundary region will result in a discontinuity of slip planes from one grain to another

Check out the Hall-Petch Equation

$$\sigma_y = \sigma_0 + Kd^{-1/2}$$

σ_y: Yield Strength [MPa]
d: Grain size [mm]
σ_0, k: Constants



Metals having small grains – relatively strong and tough at low temperatures

Metals having large grains – good creep resistance at relatively high temperatures

A fine-grained material is harder and stronger due to a greater total grain boundary area to imposed dislocation motion

Cold Work - Strain Hardening or Work Hardening

- Cold work is also known as strain hardening. It is the phenomenon whereby a ductile metal becomes harder and stronger as it is plastically deformed.

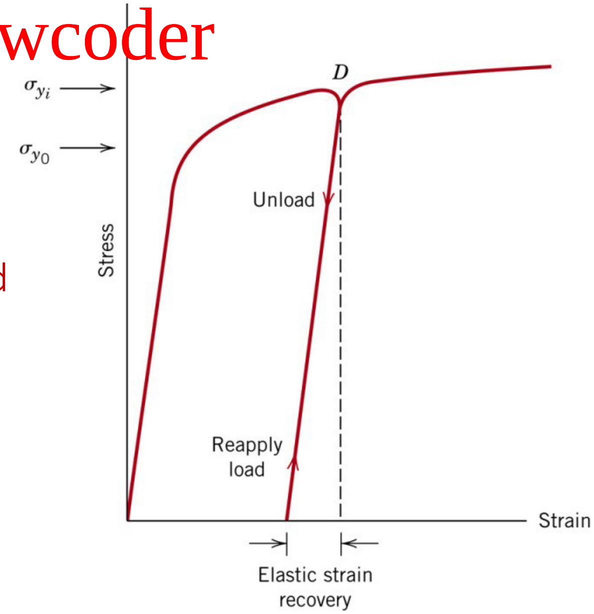
- In single crystals: dislocation movements -> plastic deformation/slip
- In polycrystalline metals: dislocation movements occur preferentially in grains with slip systems that is most favourably located relative to the load direction

- Rotation occurs to bring the grains into more favourable position, so as to keep the grain boundaries in contact
- Most grains will eventually have a

plane in the direction of deformation.

- A considerable amount of distortion will have occurred,

and the materials will have gone straining or work hardening.



How a metal becomes harder and stronger as it is plastically deformed, or work hardened. However, this effect can be removed’ by **heat treatment**

Alloying

A metal alloy is a mixture or series of metallic solid solutions or phases, composed of two or more elements

Alloys can be produced with mixtures of :

- Metals/Metals e.g., Cu-Zn (Brass)

- Metals/Non-metals e.g., Fe-C (Steel)

- Metals/Gas e.g., FeCrNiN (a Stainless Steel)

Intersolubility of elements varies from ~0% to 100%

- Al-Sn immiscible in both liquid and solid state
- Cd-Bi soluble in liquid state only
- Cu-Zn limited solubility of Zn in Cu in solid state
- Cu-Ni mutual soluble in liquid and solid state

Learning Outcome Check 4

- What properties can we determine from the tensile test?
- Name two methods to determine toughness of a material.

- How does grain size reduction result in strengthening of metals?

- How does work hardening result in strengthening of metals?

- What is an alloy?

Formation of alloys

A **useful** alloy is only formed when the elements in question are mutually soluble in the liquid state. Upon cooling, following conditions may occur:

- Insoluble in the solid state - they separate out as particles of the two pure metals.

- Complete or partial solubility in the solid state - in the former case a single solid solution forms, whilst in the latter a mixture of two different solid structures results.

- An intermetallic compound, or an intermediate phase forms in the solid state.

Constitution of Alloys

- The resulting constitution of alloys:
  - Single phase solid solution
  - Multiphase alloy
  - Multiphase alloy with precipitates
  - Highly strained metastable states

- For load bearing alloys, the required properties are a combination of **strength** and **toughness.**

- These properties are controlled to a large extent by **adjusting the structure** of the alloy to control the behaviour of **dislocations**.

- On a microstructural level this is done by affecting the **atomic lattice configurations** of the alloy.

Solid Solutions

- A solid solution forms when metals dissolve in all ratios one into the other.
- A solid state phase in which the primary element has incorporated atoms of the secondary element(s) into the primary lattice.
- Sites for the secondary element atoms can be:

  Normal primary element sites:

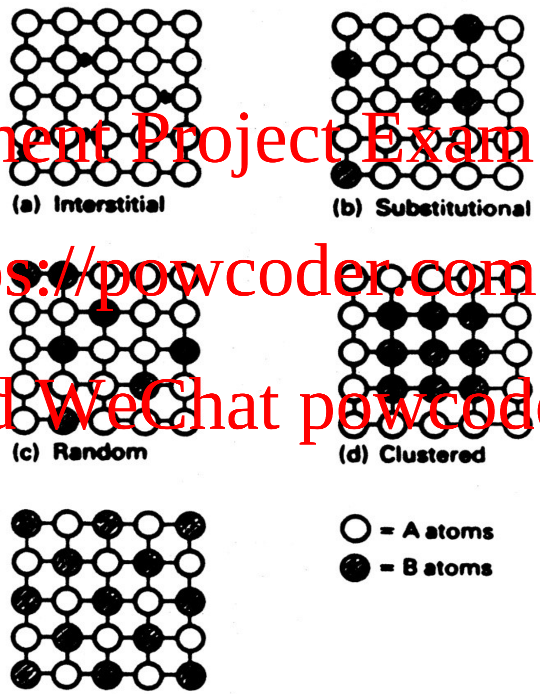
  substitutional solid solution (SSS)

  Between primary element sites:

  interstitial solid solution (ISS)

- Both SSS and ISS atoms create strain field within crystal lattice, which act to resist dislocation movement

Strengthening Mechanisms in Metallic Materials



Solid-solution structures. In *interstitial* solutions small atoms fit into the spaces between large atoms. In *substitutional* solutions similarly sized atoms replace one another. If A–A, A–B and B–B bonds have the same strength then this replacement is *random*. But unequal bond strengths can give *clustering* or *ordering*.

Substitutional Solid Solution

Several factors are known that control ranges of ***substitutional solid solubility*** in alloy systems.

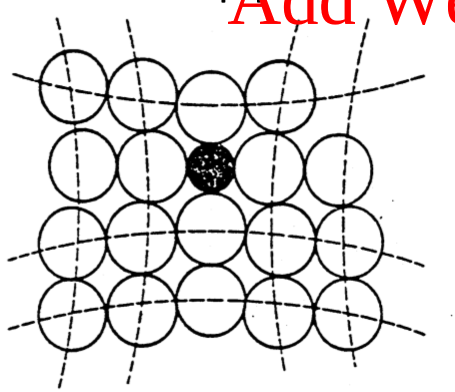
- Crystal-structure factor - as indicated above complete solid solubility of two elements is never attained unless the elements have the same type of crystal lattice structure.

- Relative size factor - the size factor is favourable for solid solution formation when the difference in atomic size is less than about 15%.

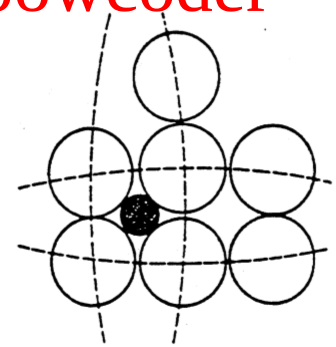
- Chemical-affinity factor - the greater the chemical affinity of two elements, the more restricted is their solid solubility. Generally, the further apart the elements are in the periodic table, the greater is their chemical affinity.

Interstitial Solid Solutions

- An **interstitial** solid solution (b) is formed when atoms of small atomic size fit into the spaces of the lattice structure of the larger atom elements.
- The best known and most important to engineers is the interstitial solution of **carbon in iron**, which results in **steel**. The more carbon atoms present the stronger the alloy, due to the distortion, which occurs interfering with the movement of dislocations on the slip planes of the alloy.



Substitutional



Interstitial

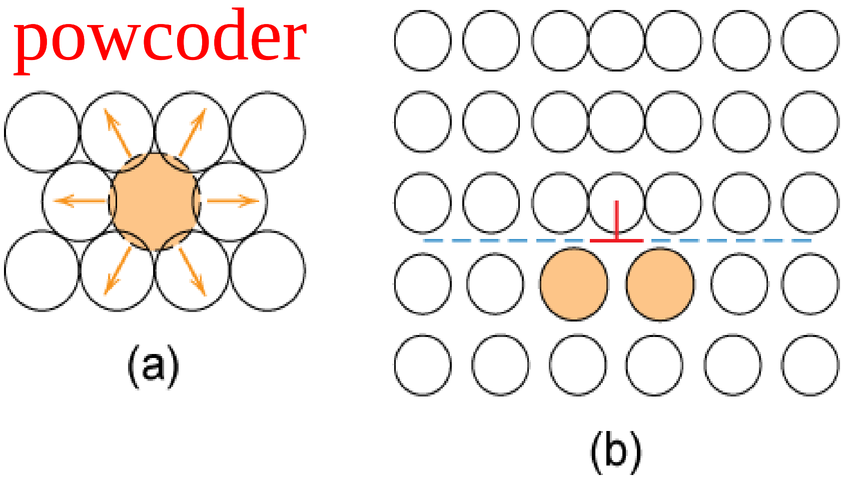
Solid Solution Strengthening

Alloys are stronger than pure metals because:

- Impurity atoms imposing lattice strains on the surrounding host atoms
- Lattice strain field interactions between dislocations and the impurity atoms result
- Dislocation movement is restricted and therefore strength is increased

(a)Compressive strains imposed on host atoms

(b) Larger impurity atoms, leading to partial cancellation of impurity-dislocation lattice strain, but a roughening of the slip plane thus causing internal friction and impeding the dislocation movement



Callister Pg.196

Next.... How to determine the optimum alloy compositions and treatments
.....Phase Equilibrium Diagrams!

Learning Outcome Check 5

- What is a solid solution?

- Distinguish between;

  a substitutional solid solution, and;

  an interstitial solid solution.

- Give three factors that would control substitutional solid solubility?

- How does alloying result in strengthening of metals?

- Give a very common engineering example of an interstitial solid solution?