Materials Science & Engineering



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Chapter 1

Introduction

The University of Jordan
Chemical Engineering Department
First Semester 2021
Prof. Yousef Mubarak

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Outlines

- What is materials science?
- Structure, Processing, & Properties
- Types of Materials
- The Materials Selection Process
- Materials Properties

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Materials Science

What is materials science? it is a continuous field of research

- Materials science or materials engineering is an interdisciplinary field involving the properties of matter and its applications to various areas of science and engineering.
- This science investigates the relationship between the structure of materials at atomic or molecular scales and their macroscopic properties.

Materials drive our society

- Stone Age - Bronze Age - Iron Age
- Now? Silicon Age? Polymer Age?

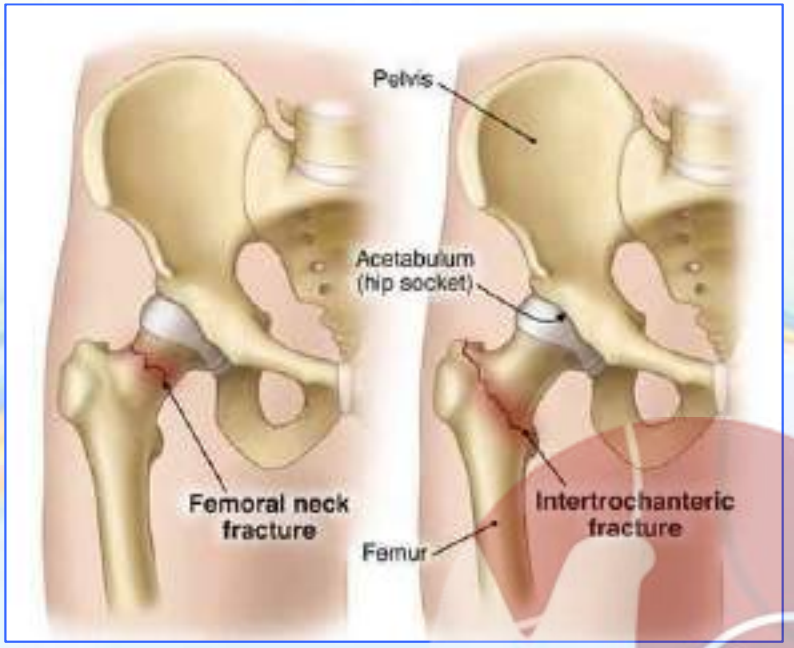
(*) while doing imperfection not all the properties will be enhanced.

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Example – Hip Implant

- With age or certain illnesses joints deteriorate.
- Particularly those with large loads (such as hip).

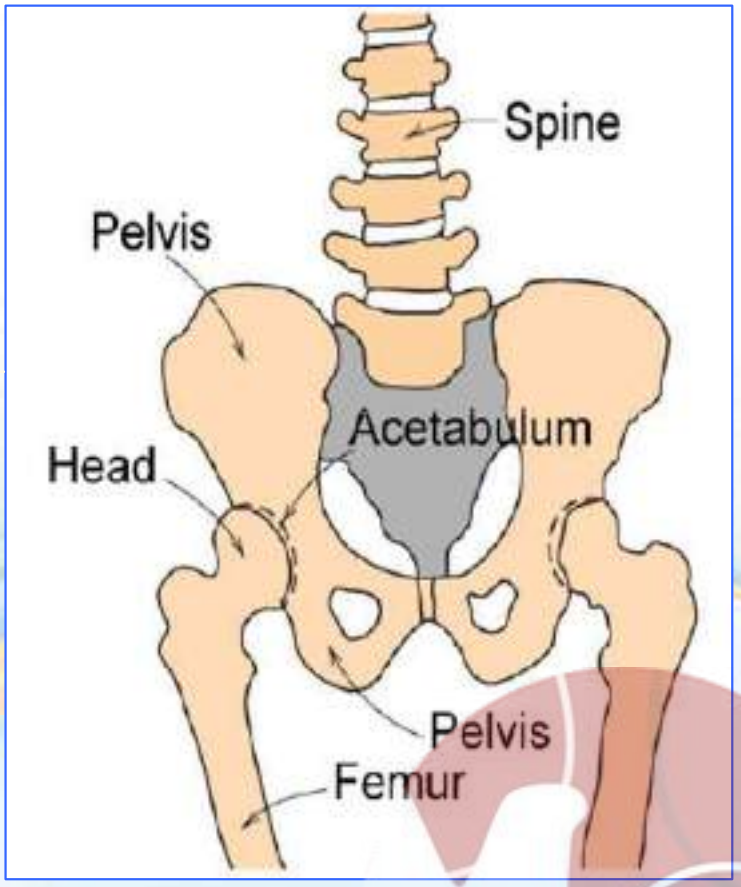




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Requirements

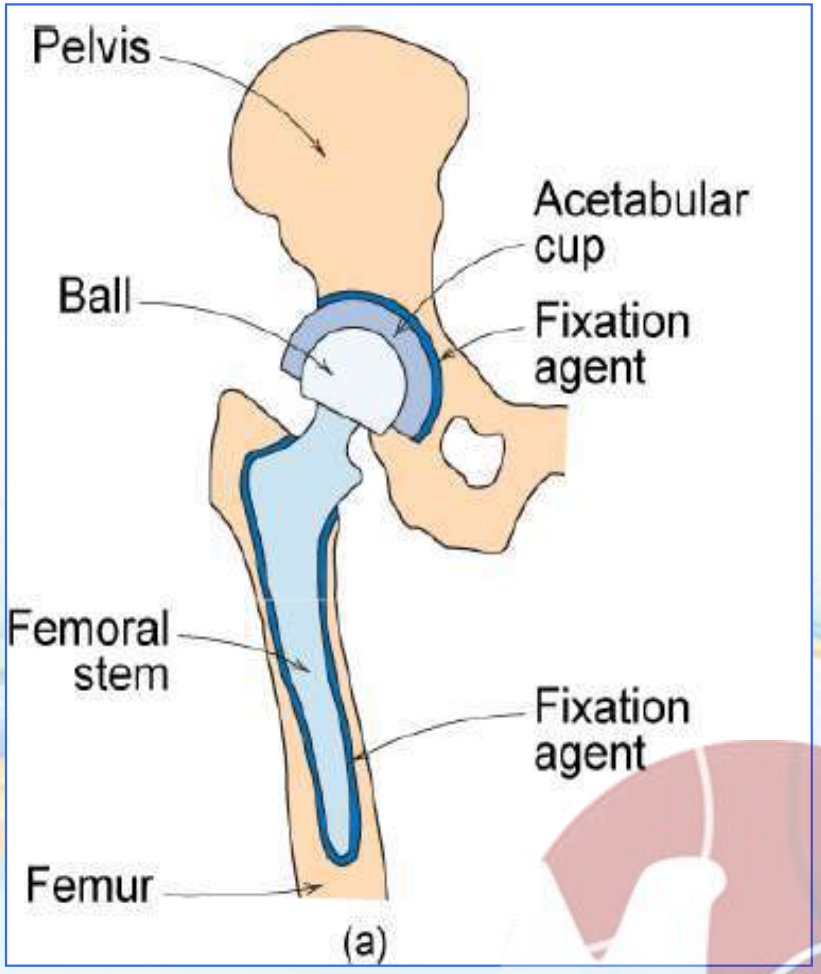
- Mechanical strength (many cycles) => في تطبيقات تحتاج أكثر من مرة أو أقل تحتاج صلابة (durability) وكمان كم يدوم تحمل لازم تناسبي
- Good lubricity
  - ↳ يقلل الاحتكاك بين الأجزاء (hardness)
- Biocompatibility The body should not reject it
- Light weight => must be the weight of the material compared to the weight of the bone (for example)
- Machinability يقصد بها سهولة تشكيل المادة أو تصنيعها ↳ rolling technique is the most common one in the industrey.



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The main factor about machinability is the material construction (how the material will be made of) → plastic, iron —
e.g:- welding, casting, CLC — etc. + how we will fix this material at the place we want.

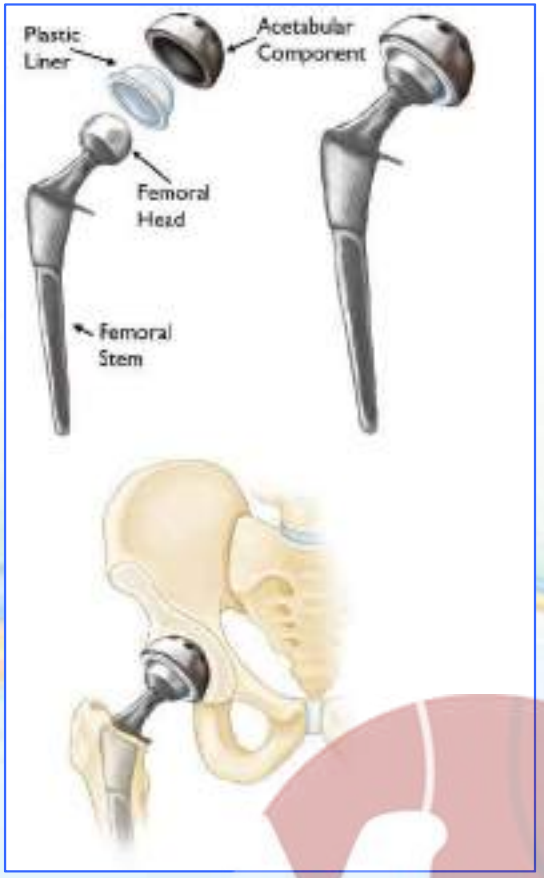




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Key problems to overcome

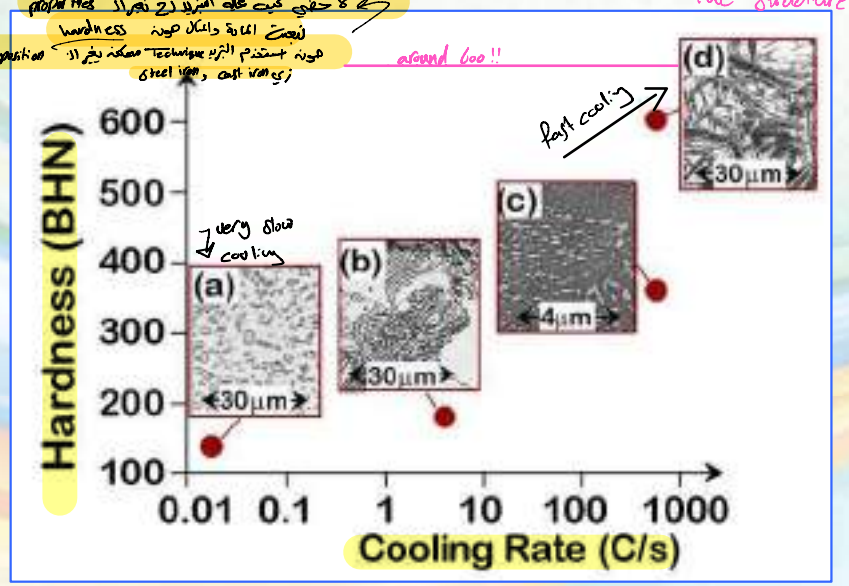
- Fixation agent to hold acetabular cup.
- Cup lubrication material.
- Femoral stem – fixing agent ("glue").
- Must avoid any debris in cup.

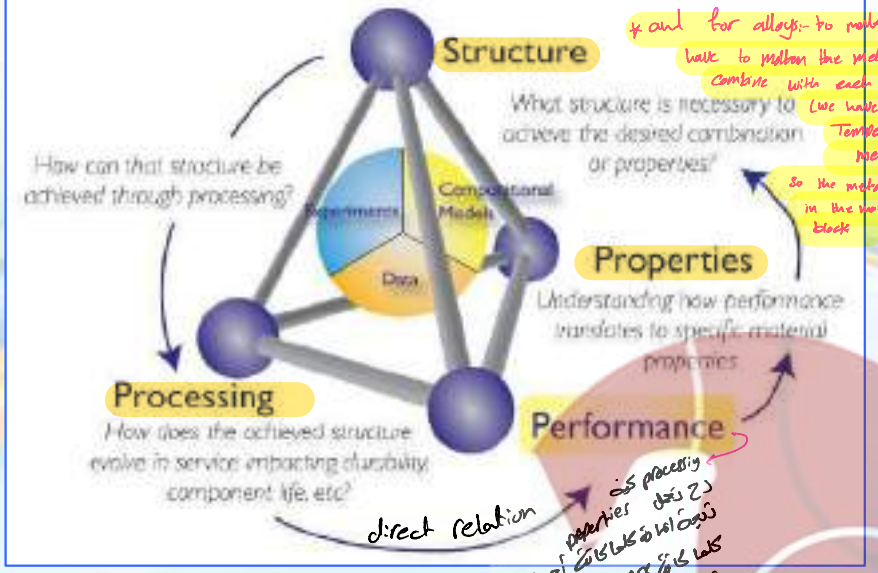


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Structure, Processing,& Properties

- Properties depend on structure:
  ex: hardness vs structure of steel
- Processing can change structure:
  ex: structure vs cooling rate of steel





Types of Materials

1. Metals

weakest @ room temperature is Mercury, strongest is the tungsten

- Strong, ductile → can be stretched.
- High thermal & electrical conductivity
- Opaque, reflective. → not transparent

2. Polymers/plastics

group of mers

⇒ plastic vs polymers?
polymers are the raw material of the plastic
the plastic are the end product
Polymers => are hydrocarbons (having covelents bonds) → non metal + non metal

has a very high mw (in thousands!) such as polyethylene.

- Covalent bonding → compared with metallics they are very weak
- Soft, ductile, low strength, low density
- Thermal & electrical insulators → we can convert it to a conductive polymer by doing imperfiction
- Optically translucent or transparent. → as the material crystalyne ↑ the transparentor and as it more amorphous the transparent will be ↑

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3. Ceramics

- Ionic bonding (refractory)
- Compounds of metallic & non-metallic elements (oxides, carbides, nitrides, sulfides)
- Brittle, glassy → it can't be bended.
- Elastic non-conducting (insulators) → if we do a tension test the ceramic will resist then broke

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The Materials Selection Process

1. Pick application

- Determine required Properties.
- Properties: mechanical, electrical, thermal, magnetic, optical, and deteriorative.

2. Properties

- Identify candidate materials
- Material: structure, composition

3. Material

- Identify required Processing
- Processing: changes structure and overall shape

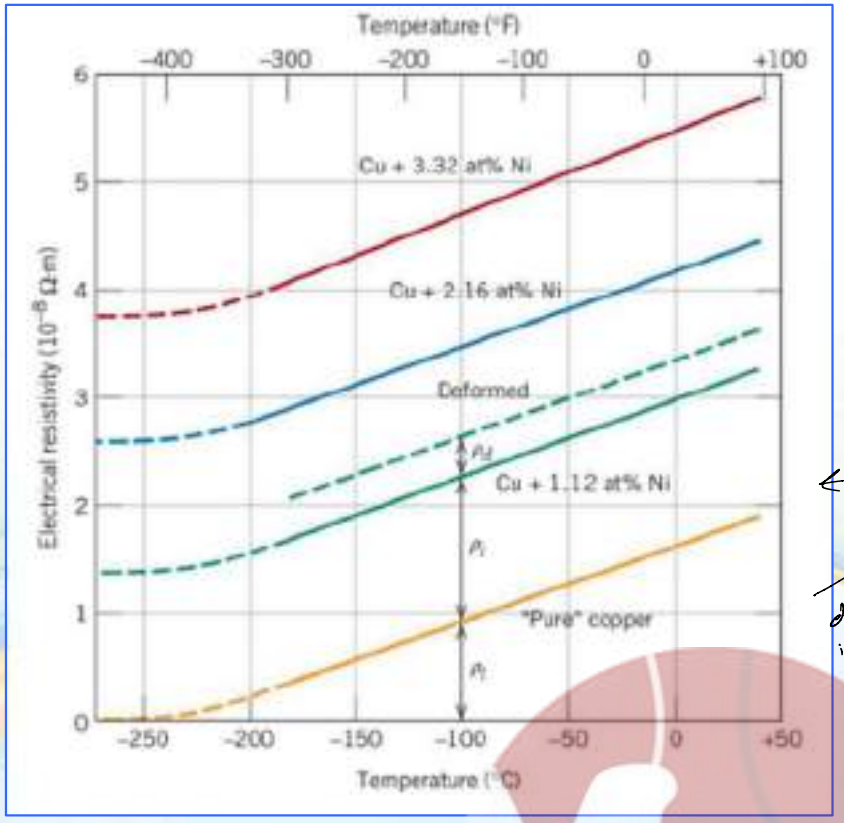
Ex: casting, sintering, vapor deposition, doping, forming, joining, and annealing.

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ELECTRICAL

Electrical Resistivity of Copper:

- ✓ Adding "impurity" atoms to Cu increases resistivity.
  - ↗ doing imperfection (deviation from its pure)
- ✓ Deforming Cu increases resistivity.



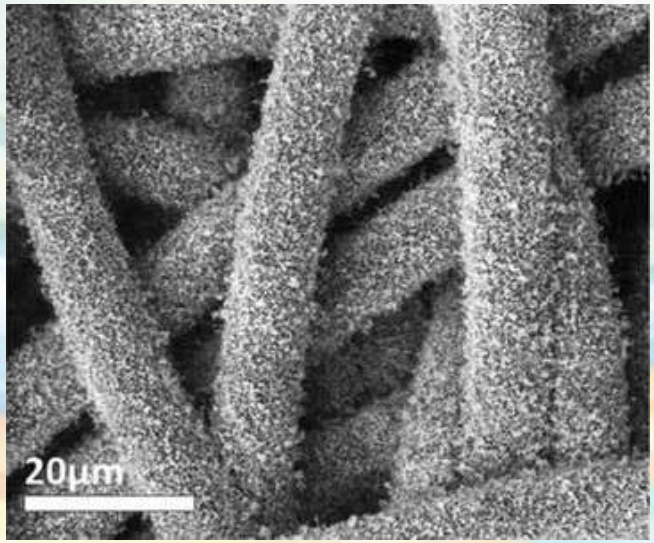
doing imperfection of Cu by adding Ni

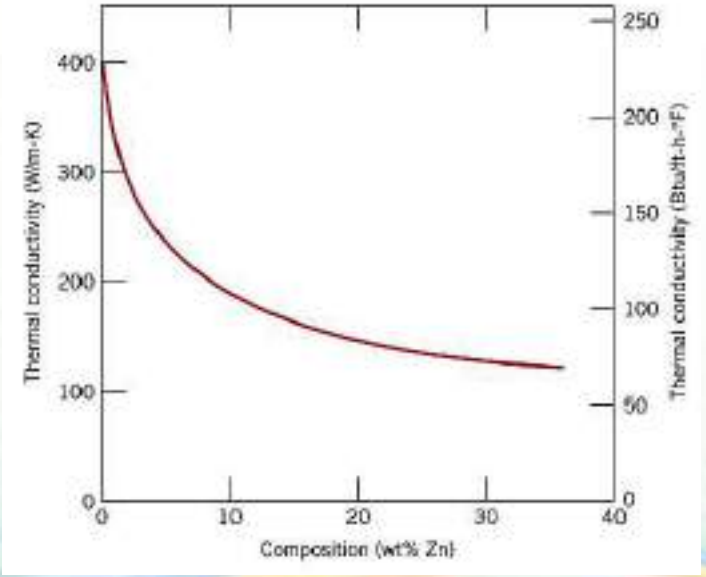
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THERMAL

Shuttle Tiles:

- Silica fiber insulation offers low heat conduction.





Thermal Conductivity of Copper:

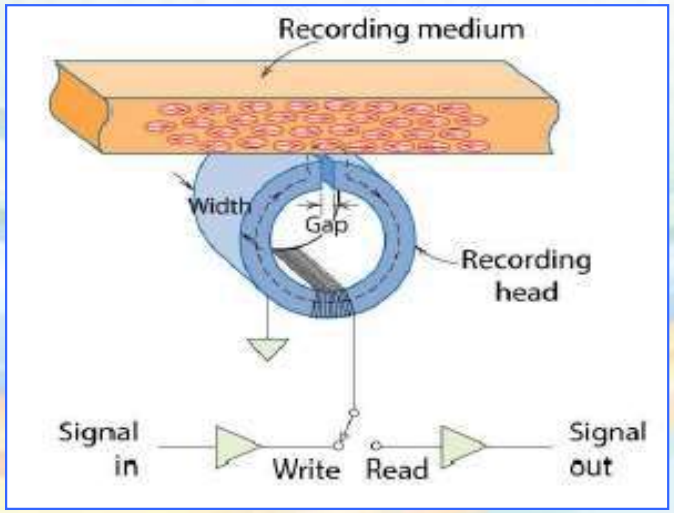
- It decreases when you add zinc.

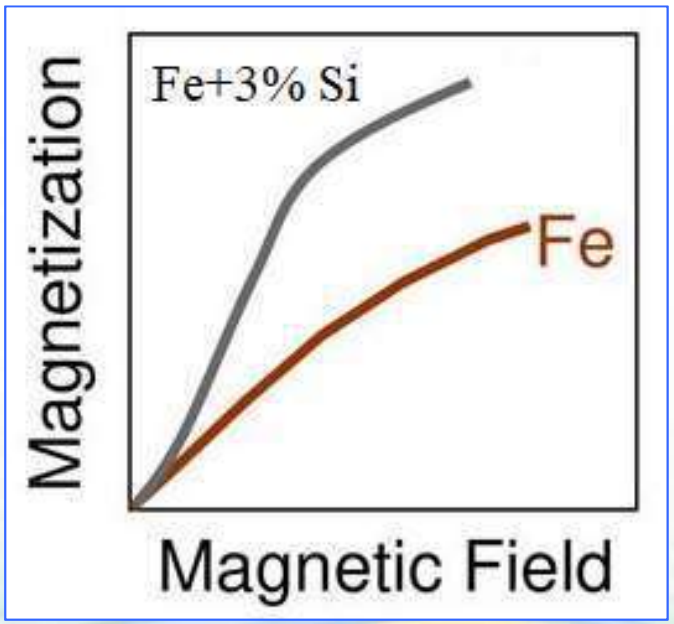
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MAGNETIC

Magnetic Storage:

- Recording medium is magnetized by recording head.





Magnetic Permeability

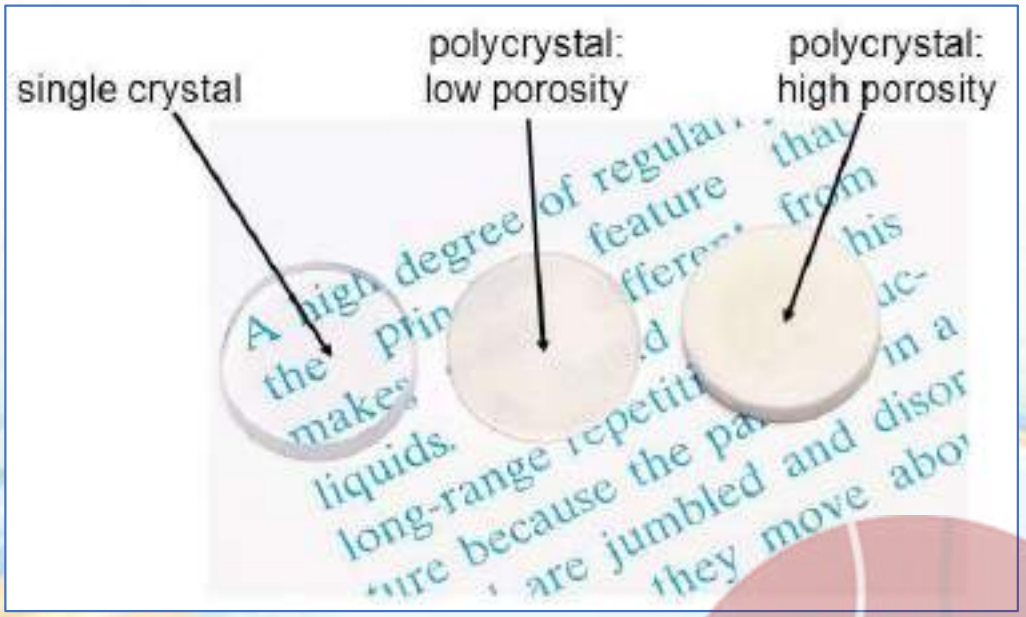
- Adding 3 % Si makes Fe a better recording medium

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OPTICAL

Transmittance:

- Aluminum oxide may be transparent, translucent, or opaque depending on the material structure.



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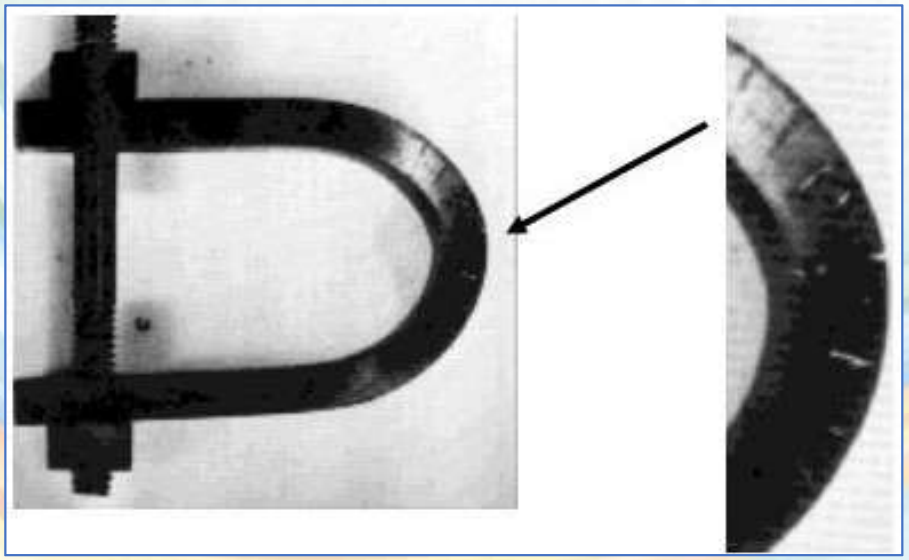
DETERIORATIVE

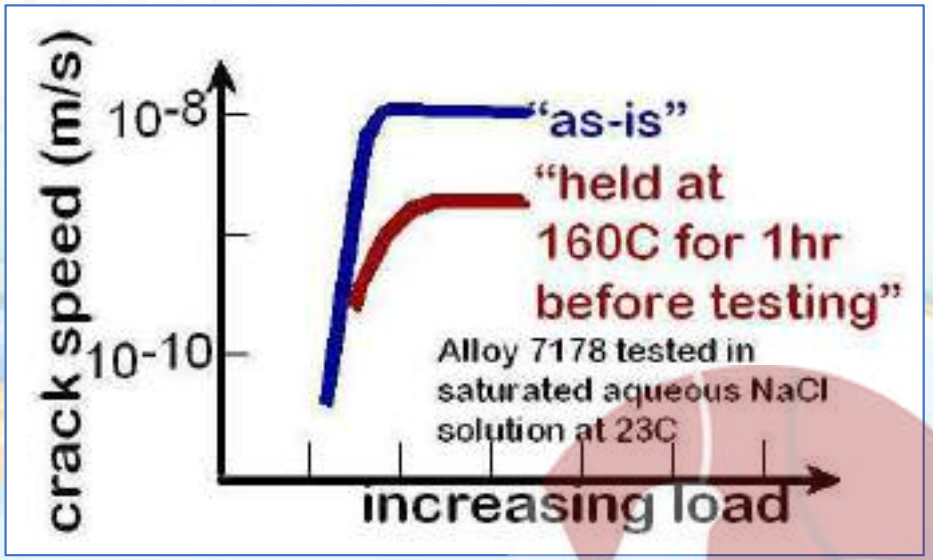
Stress & Saltwater:

- *causes cracks*

Heat treatment:

- *slows crack speed in salt water.*





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Chapter 2

Atomic Structure

The University of Jordan
Chemical Engineering Department
First Semester 2021
Prof. Yousef Mubarak

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Outline

1- Review of Atomic Structure

- Electrons, Protons, Neutrons.
- Atomic Bonding in Solids.
- Periodic Table.
- Primary Interatomic Bonds .
- Secondary Bonding (Van der Waals).

2- Molecules and Molecular Solids

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Review of Atomic Structure

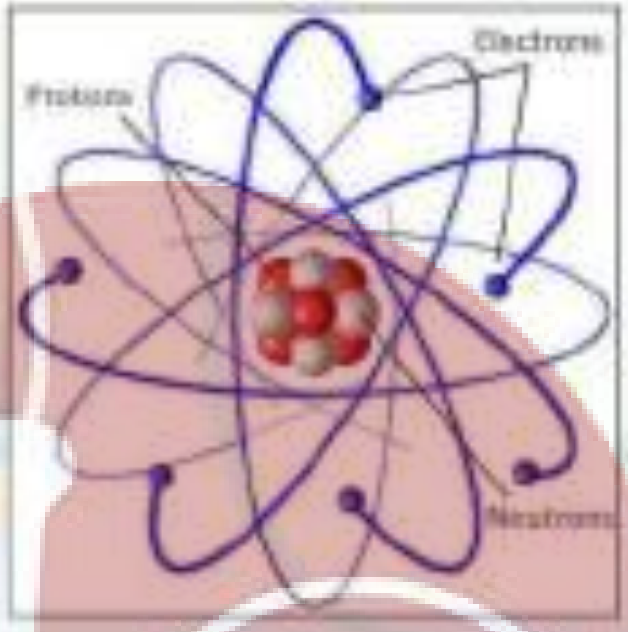
What are atoms?

- Atoms are the basic building blocks of matter that make up everyday objects.
- Atoms are made out of three basic particles:

1. Protons – carry a positive charge
2. Neutrons – carry no charge

✓ Protons and Neutrons join together to form the Nucleus – the central part of the atom

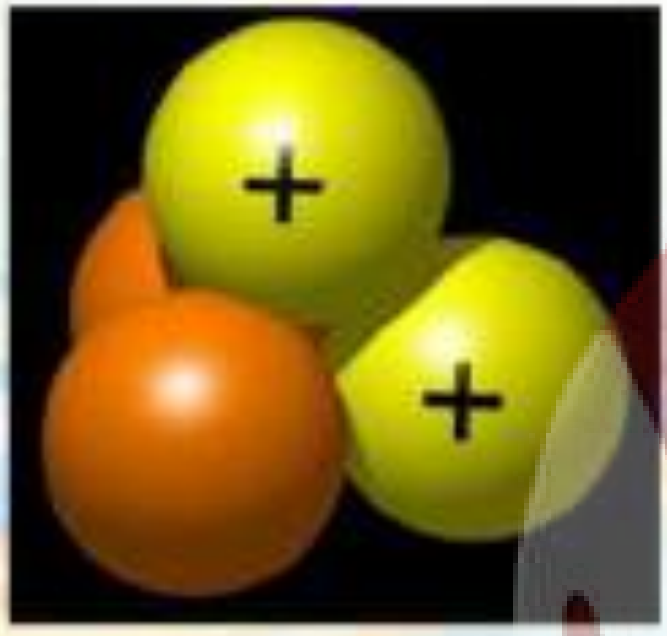
3. Electrons – carry a negative charge and circle the nucleus

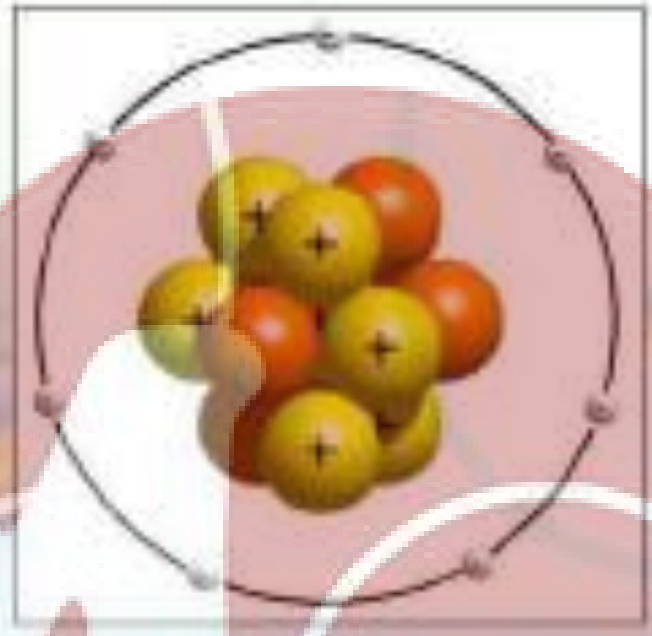


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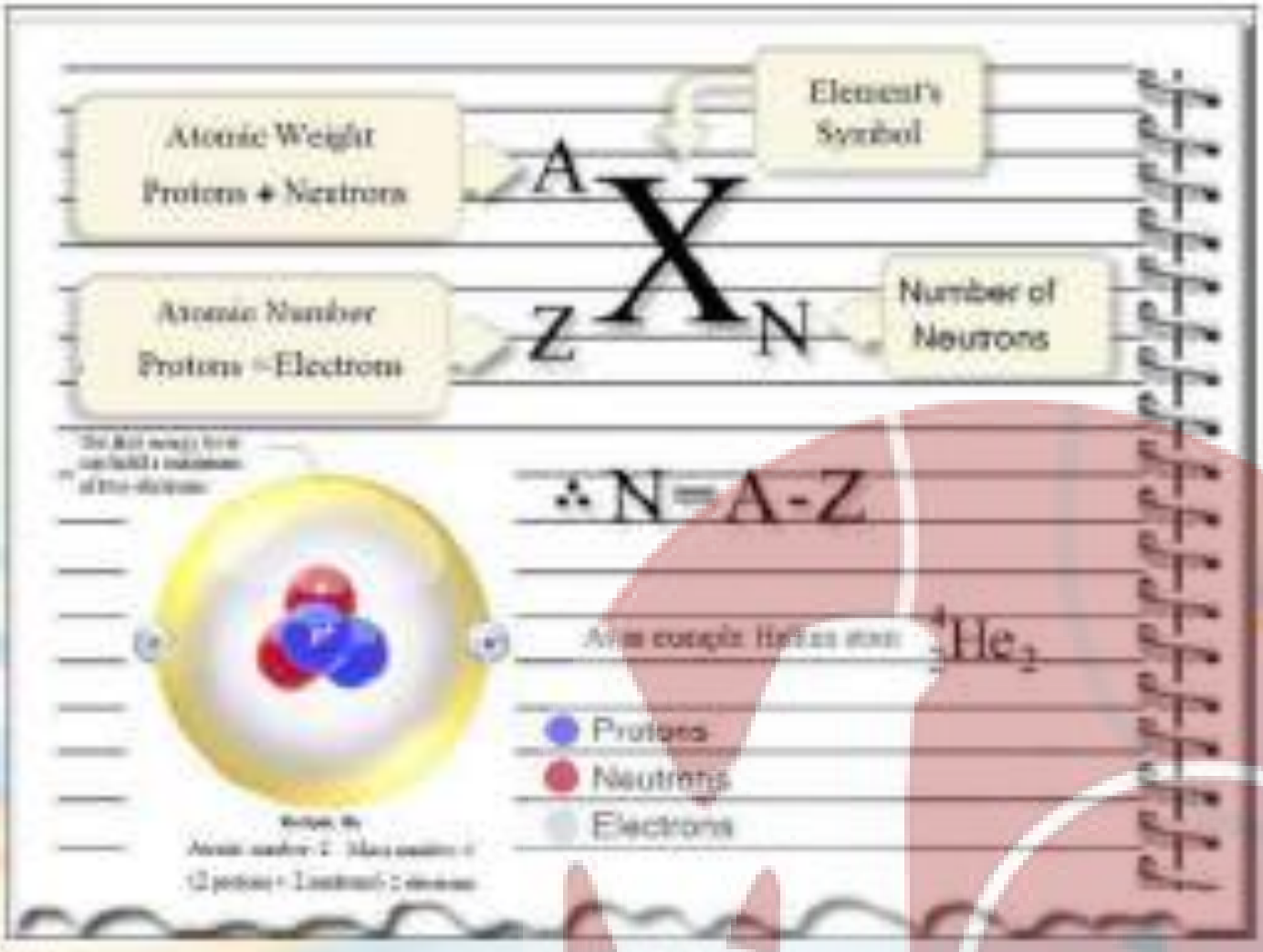
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- *The nucleus is the massive center of the atom. It was discovered in 1911, but it took scientists another 21 years of experimenting to identify its parts.*





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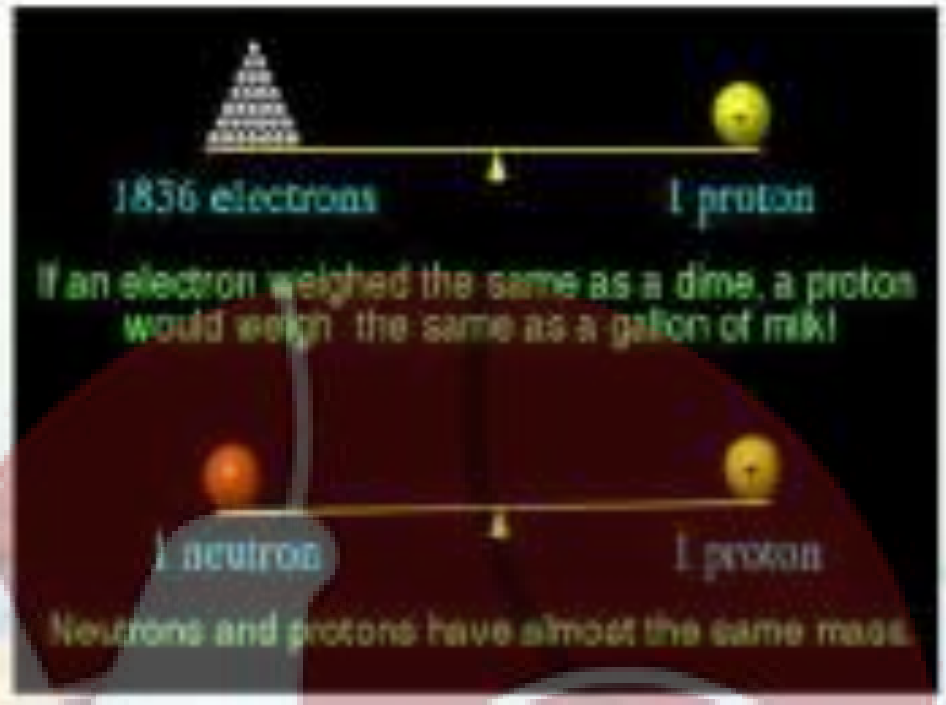
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Charges:

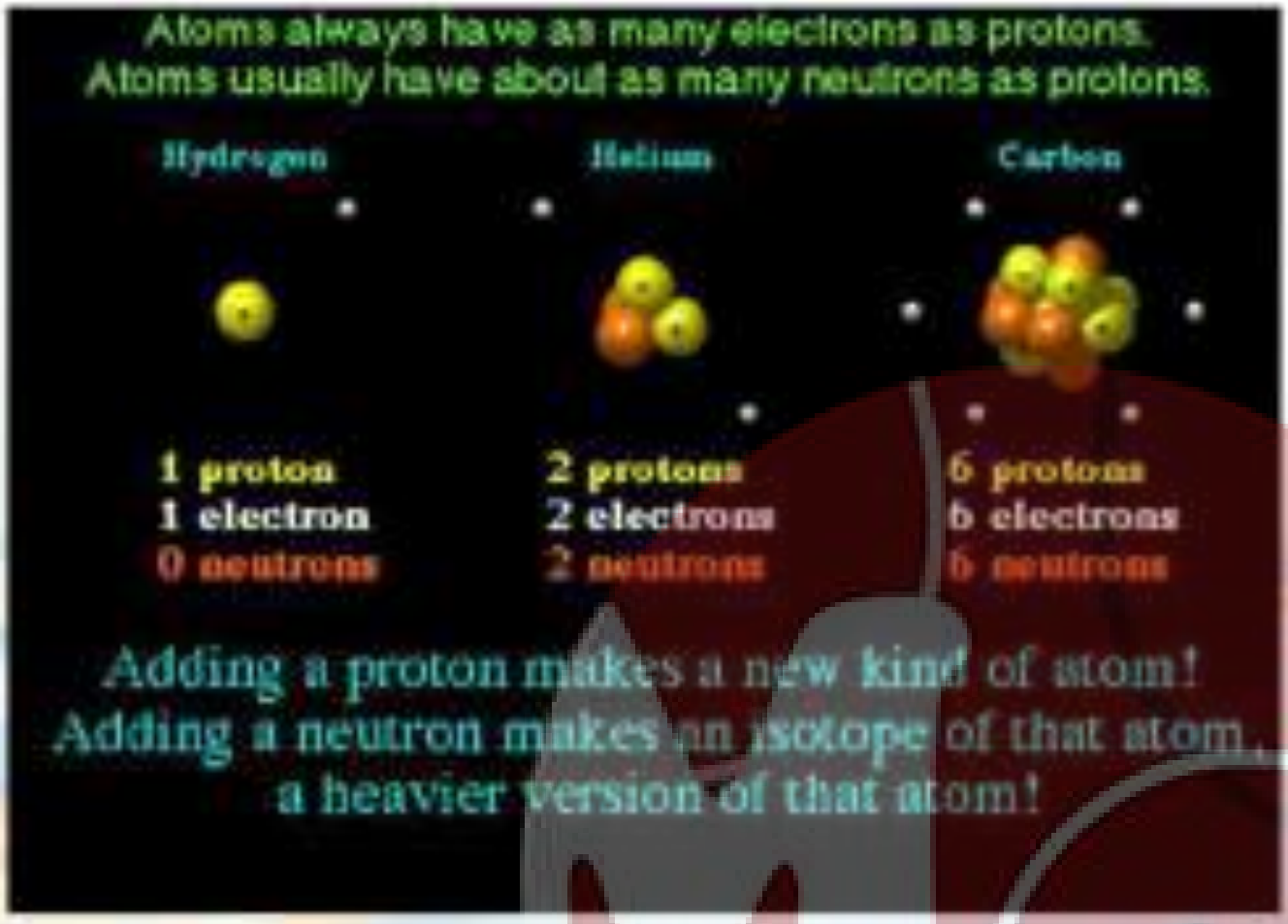
- *Electron's and Proton's charges are of the same magnitude, 1.602 × 10^{-19} Coulomb.*

Masses:

- *Protons and Neutrons have the same mass, 1.67 × 10^{-27} kg.*
- *Mass of an electron is much smaller, 9.11 × 10^{-31} kg and can be neglected in calculation of atomic mass.*



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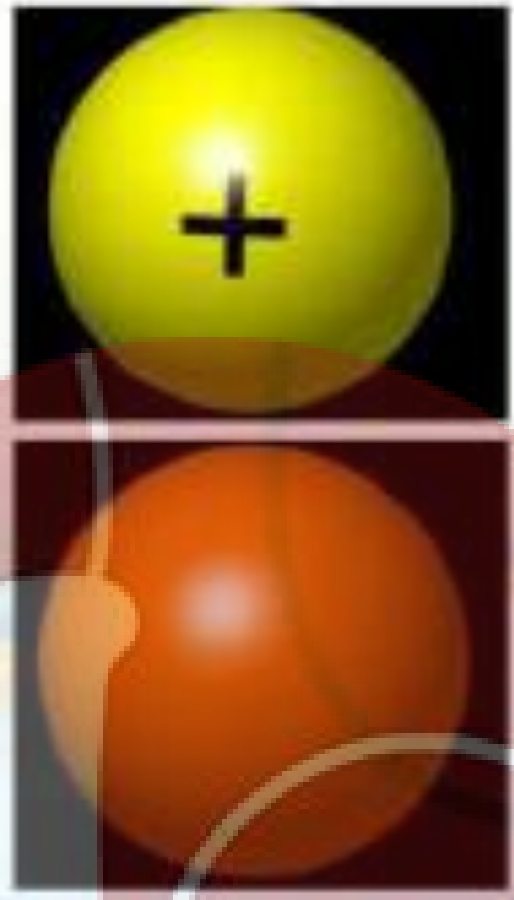
adding electron → does not change the nature of the atom

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- *Scientists thought there was nothing smaller than the proton in the nucleus of the atom.*

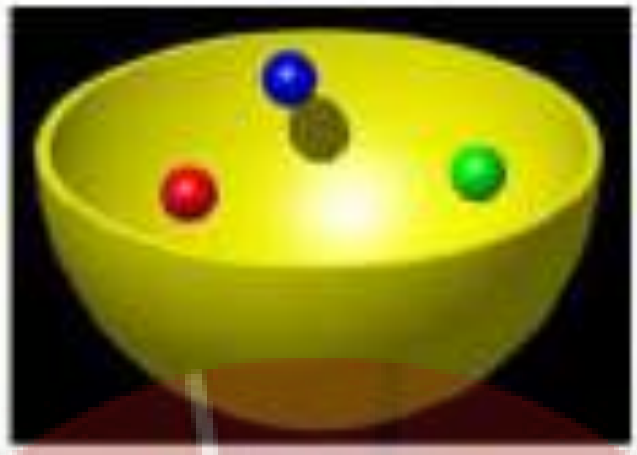
- *Scientists discovered the neutron in 1932. They thought that there was nothing smaller in the atom's nucleus?*

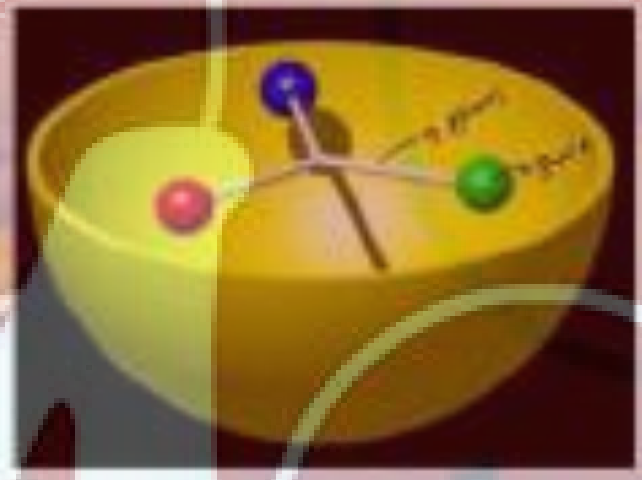


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- In 1968, scientists discovered new particles inside the proton. They called these particles quarks.

- There are three quarks in each proton. The quarks are held to each other by other particles called gluons.

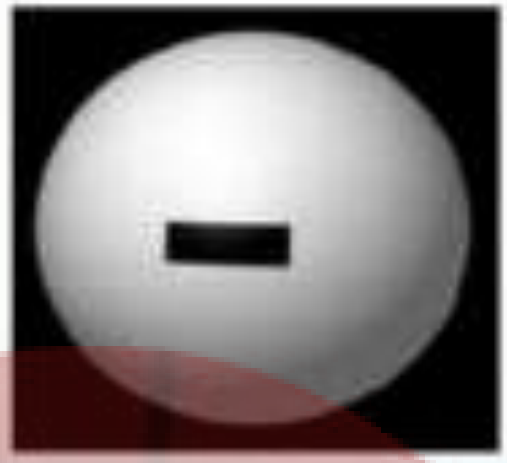




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- Electrons are extremely small and very light.
- It is easy to strip off electrons of atoms and use them for electrical power and in devices like television sets.
- Electrons can be used to probe inside of atoms. Higher energy electrons can detect smaller features inside of atoms. Scientists learn about the inside of atoms by watching how electrons bounce off the atom, and by how the atom changes as a result of being hit by an electron.





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Number of Atoms

- The number of atoms per cm^3, n, for material of density d (g/cm^3) and atomic mass M (g/mol) is:

$$n = \frac{N_{av} d}{M}$$

where N_{av} is Avogadro's number = 6.022×10^{23} atms/mol

- Mean distance between atoms

$$L = \left(\frac{1}{n}\right)^{1/3}$$

Example:

Diamond (carbon): $d = 3.5\ g/cm^3$, $M = 12\ g/mol$

$n = 6 \times 10^{23}\ atoms/mol \times 3.5\ g/cm^3 / 12\ g/mol$

$= 17.5 \times 10^{22}\ atoms/cm^3$

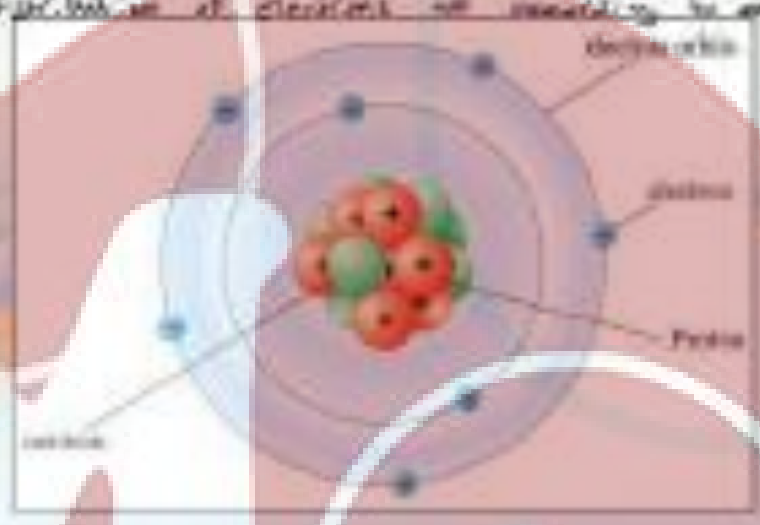
$L = (1/(17.5 \times 10^{22}))^{1/3} = 0.179\ nm$

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Electrons in Atoms

- The electrons form a cloud around the nucleus, of radius of 0.05 – 2 nm.
- This "Bohr" picture looks like a mini planetary system. But quantum mechanics tells us that this analogy is not Correct.
- Electrons move not in circular orbits, as in popular drawings, but in 'fuzzy' orbits.



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- One cannot tell how it moves, but only say what is the probability of finding it at some distance from the nucleus.
- Valence electrons determine all of the following properties:
  - ✓ Chemical.
  - ✓ Electrical.
  - ✓ Thermal.
  - ✓ Optical.
- Each orbital at discrete energy level determined by quantum numbers.

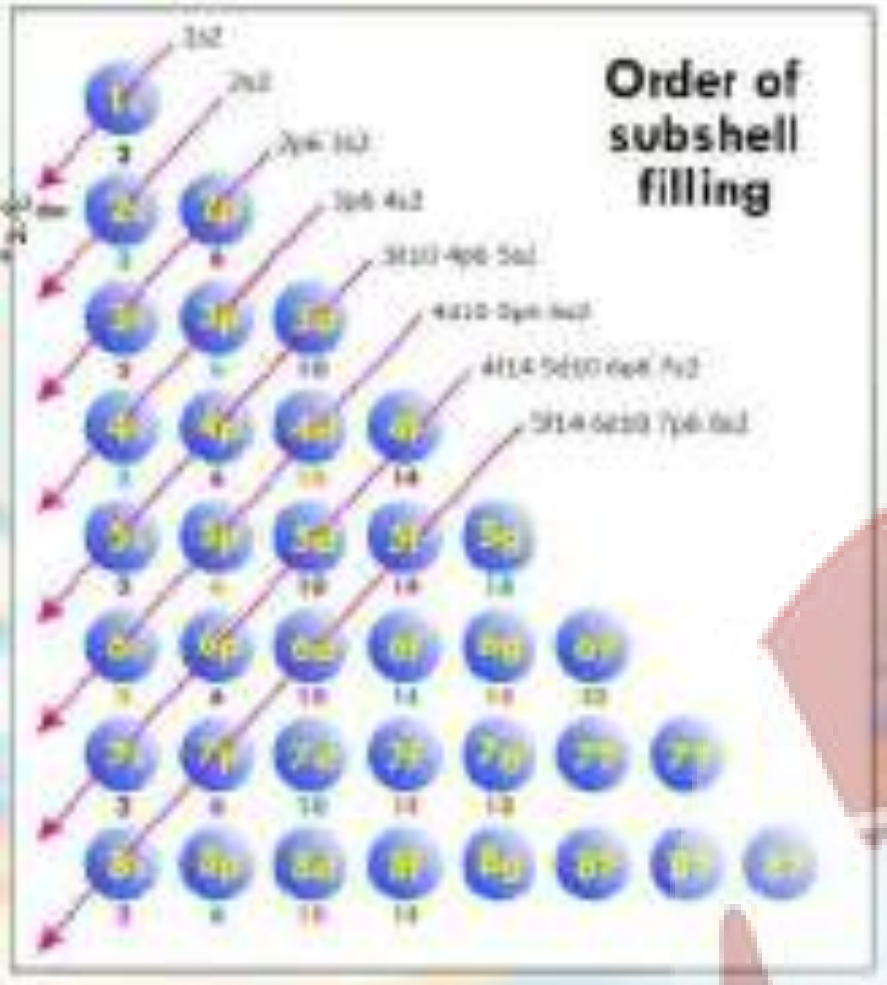
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- *The number of available electron states in some of the electron shells and subshells*

Principal Quantum number n	Shell designation	Subshells	Number of States	Electrons per Subshell	Electrons per Shell
1	K	S	1	2	2
2	L	S	1	2	8
		P	3	6	
3	M	S	1	2	18
		P	3	6	
		D	5	10	
4	N	S	1	2	32
		P	3	6	
		D	5	10	
		F	7	14	

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Subshells by energy:

1s,2s,2p,3s,3p,4s,3d,4p,5s,4d,5p,6s,4f,...

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➢ *Most elements: Electron configuration not stable.*

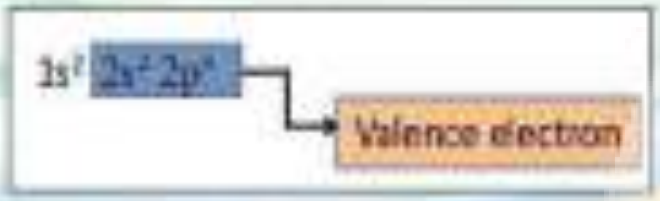
Element	Atomic #	Electron configuration
Hydrogen	1	$1s^1$
Helium	2	$1s^2$ (stable)
Lithium	3	$1s^2 2s^1$
Beryllium	4	$1s^2 2s^2$
Boron	5	$1s^2 2s^2 2p^1$
Carbon	6	$1s^2 2s^2 2p^2$
...	...	...
Neon	10	$1s^2 2s^2 2p^6$ (stable)
Sodium	11	$1s^2 2s^2 2p^6 3s^1$
Magnesium	12	$1s^2 2s^2 2p^6 3s^2$
Aluminum	13	$1s^2 2s^2 2p^6 3s^2 3p^1$
...	...	...
Argon	18	$1s^2 2s^2 2p^6 3s^2 3p^6$ (stable)
...	...	...
Krypton	36	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$ (stable)

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Valence Electron

- Valence electrons - those in unfilled shells.
- Filled shells more stable.
- Valence electrons are most available for bonding and tend to control the chemical properties.

Example: O (atomic number = 8)





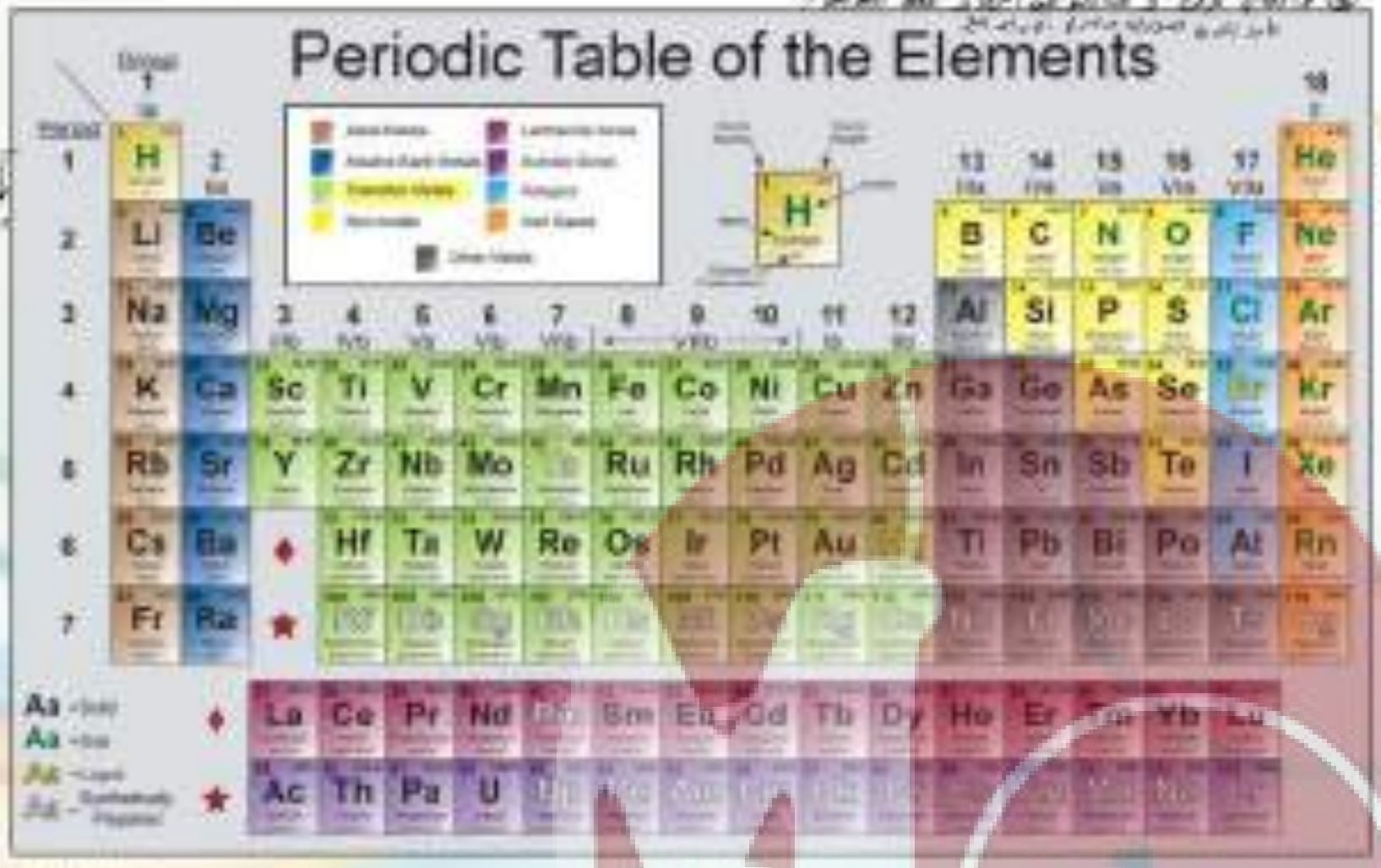
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The Periodic Table

- Electrons that occupy the outermost filled shell (the valence electrons) they are responsible for bonding.
- Electrons fill quantum levels in order of increasing energy (due to electron penetration).
- Example: Iron, Fe = 26: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 4s^2$. Elements in the same column (Elemental Group) share similar properties.
- Group number indicates the number of electrons available for bonding.
  - ✓ 0: Inert gases (He, Ne, Ar...) have filled subshells: chemically inactive.
  - ✓ I A: Alkali metals (Li, Na, K...) have one electron in outermost occupied s subshell - eager to give up electron - chemically active.
  - ✓ VII A: Halogens (F, Br, Cl...) missing one electron in outermost occupied p shell - want to gain electron - chemically active.

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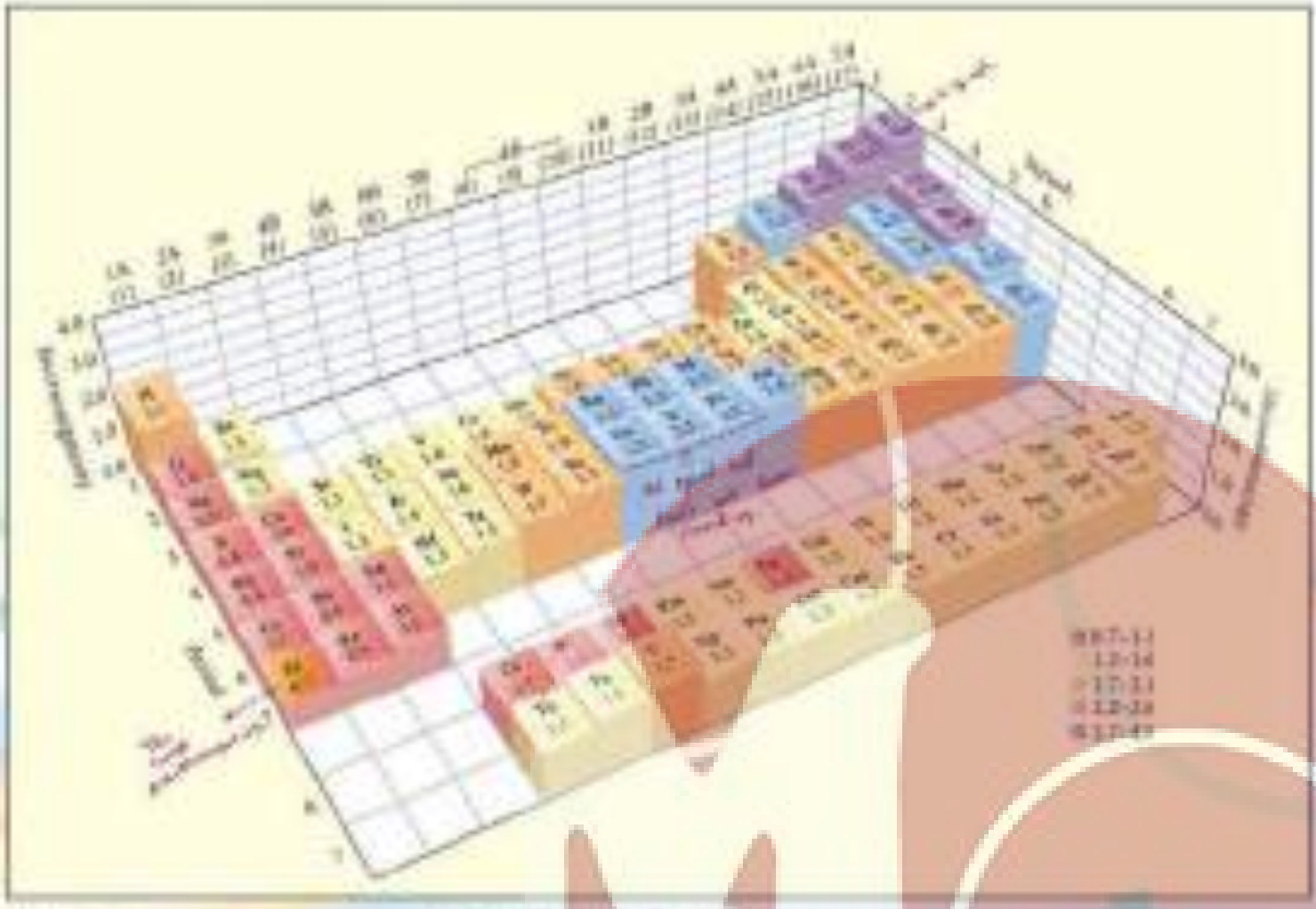


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The Electronegativity Values

- **Electronegativity** - a measure of how willing atoms are to accept electrons.
  - Subshells with one electron - low electronegativity
  - Subshells with one missing electron - high electronegativity.
  - Electronegativity increases from left to right in the periodic table.
  - Metals are electropositive - they can give up their few valence electrons to become positively charged ions.
  - Electronegativity ranges from 0.7 to 4.0

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- To calculate Pauling electronegativity for an element, it is necessary to have data on the dissociation energies of at least two types of covalent bond formed by that element.
- The difference in electronegativity between atoms A and B is given by:

$$\chi_A - \chi_B = eV^{-1/2}\sqrt{E_d(AB) - \frac{|E_d(AA) + E_d(BB)|}{2}}$$

where:

The dissociation energies, E_d of the A-B, A-A and B-B bonds are expressed in electron volts, the factor $(eV)^{-1/2}$ being included to ensure a dimensionless result.

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Example:

Calculate the difference in Pauling electronegativity between hydrogen and bromine if the dissociation energies: H-Br, 3.79 eV; H-H, 4.52 eV; Br-Br 2.00 eV.

Solution:

Note that 1 kcal/mol = 4.3363×10^{-2} eV

$$x_A - x_B = (1.602 \times 10^{-19})^{-1/2} \sqrt{\left(3.79 - \left[\frac{4.52 + 2.00}{2}\right]\right) \times 1.602 \times 10^{-19}}$$

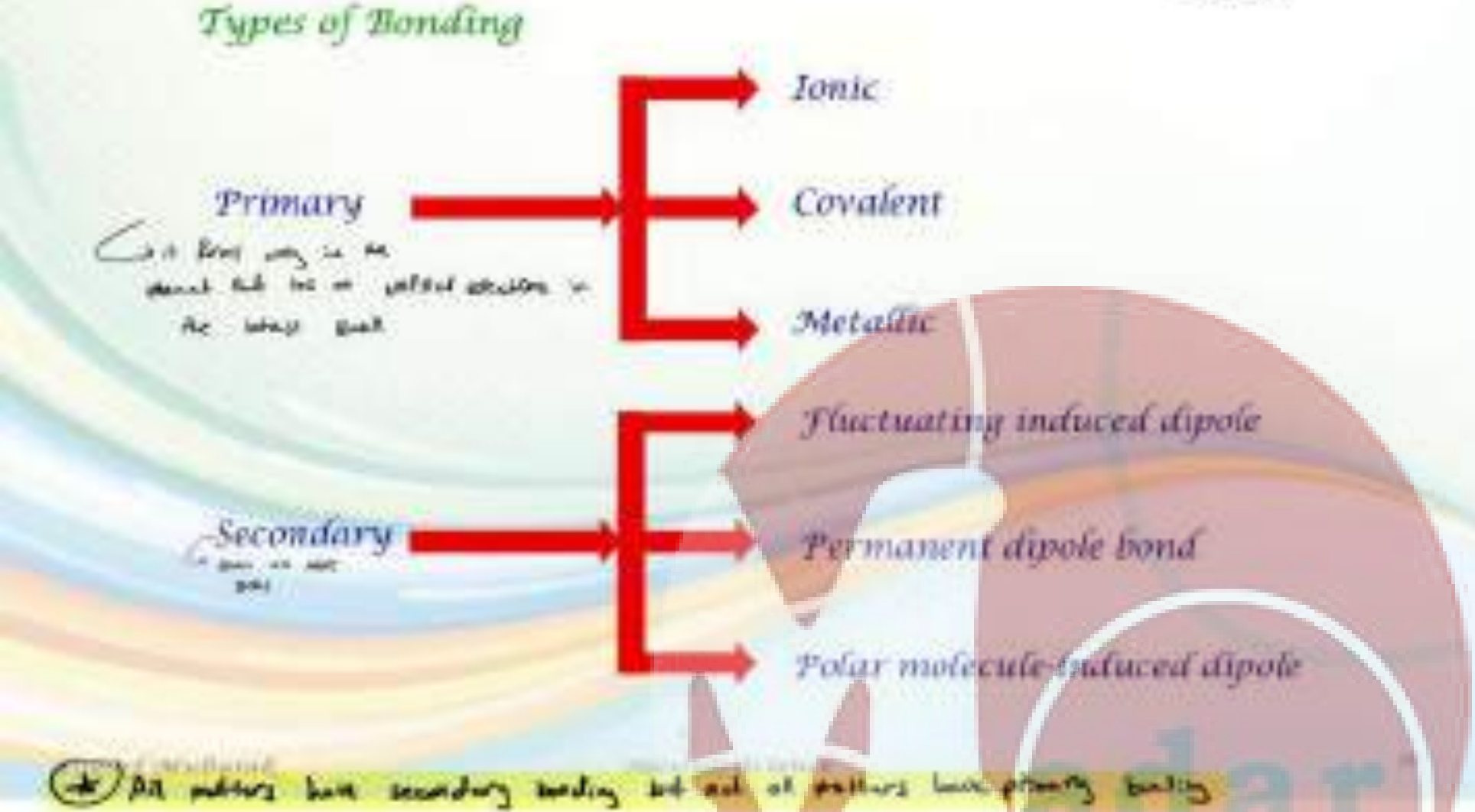
$x_A - x_B = 0.736$



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⇒ we don't have to mention Secondary Bonding if the primary bonding exist in the matter



(*) All matters have secondary bonding but not all matters have primary bonding

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it's not an absulote attraction .. why?
because both elements (the metal and the non metal) have a positive charge in the nucleus so there is also a repulsive force to make sure that both element will not collapse.

Also there are an equilibrium between these two forces from the center to the center between to elements to make sure to not be seperated or collapsed.

- high Boiling and melting points
- form as crystals
- conduct electricity if dissolved in water and exsist as ions.
- Brittle and easily broken into a small pieces.

Ionic Bonding

Formation of ionic bond: (metal + non metal)

Based on acceptance and donation (high difference in electronegativity)

1- Mutual ionization occurs by electron transfer (remember electronegativity table) ⇒ عشان هيك هذه الي بطلة تكون بين metal + non metal

- ✓ Ion = charged atom
- ✓ Anion = negatively charged atom ⇒ most of them are salts
- ✓ Cation = positively charged atom ⇒ most of them are salts

2- Ions are attracted by strong columbic interaction (very strong.) ⇝ most of them are in solid state

- ✓ Oppositely charged atoms attract
- ✓ An ionic bond is non-directional (ions may be attracted to one another in any direction

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Ionic Bonding

The size will decrease it will shrink

The size will increase "expand"

Metal

Nonmetal

Donates electrons

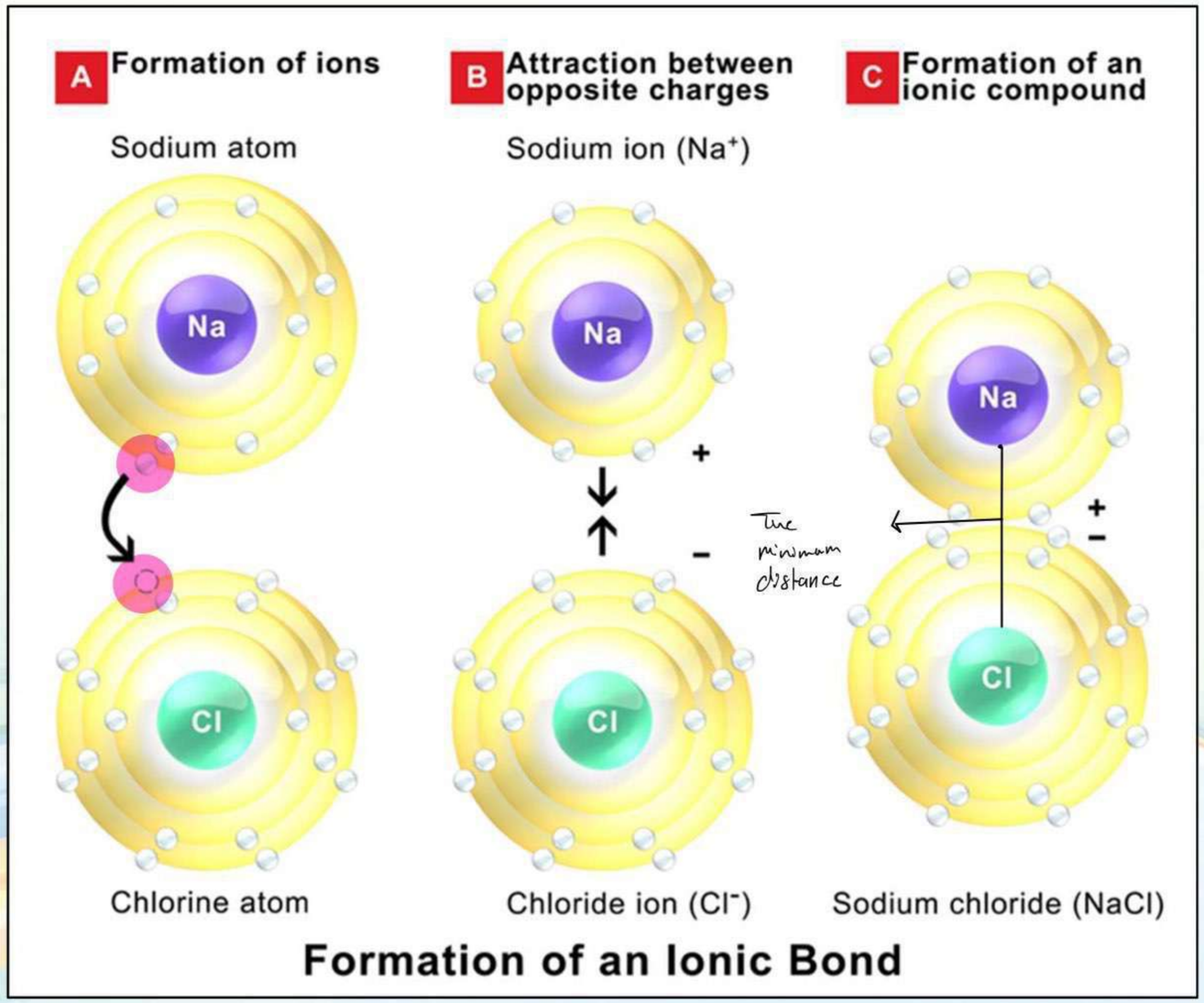
Accepts electrons

Dissimilar electronegativities

Example: NaCl

Na $1s^2\ 2s^2\ 2p^6\ 3s^1$ Cl $1s^2\ 2s^2\ 2p^6\ 3s^2 3p^5$

Na^{1+} $1s^2\ 2s^2\ 2p^6$ Cl^{1-} $1s^2\ 2s^2\ 2p^6\ 3s^2 3p^6$



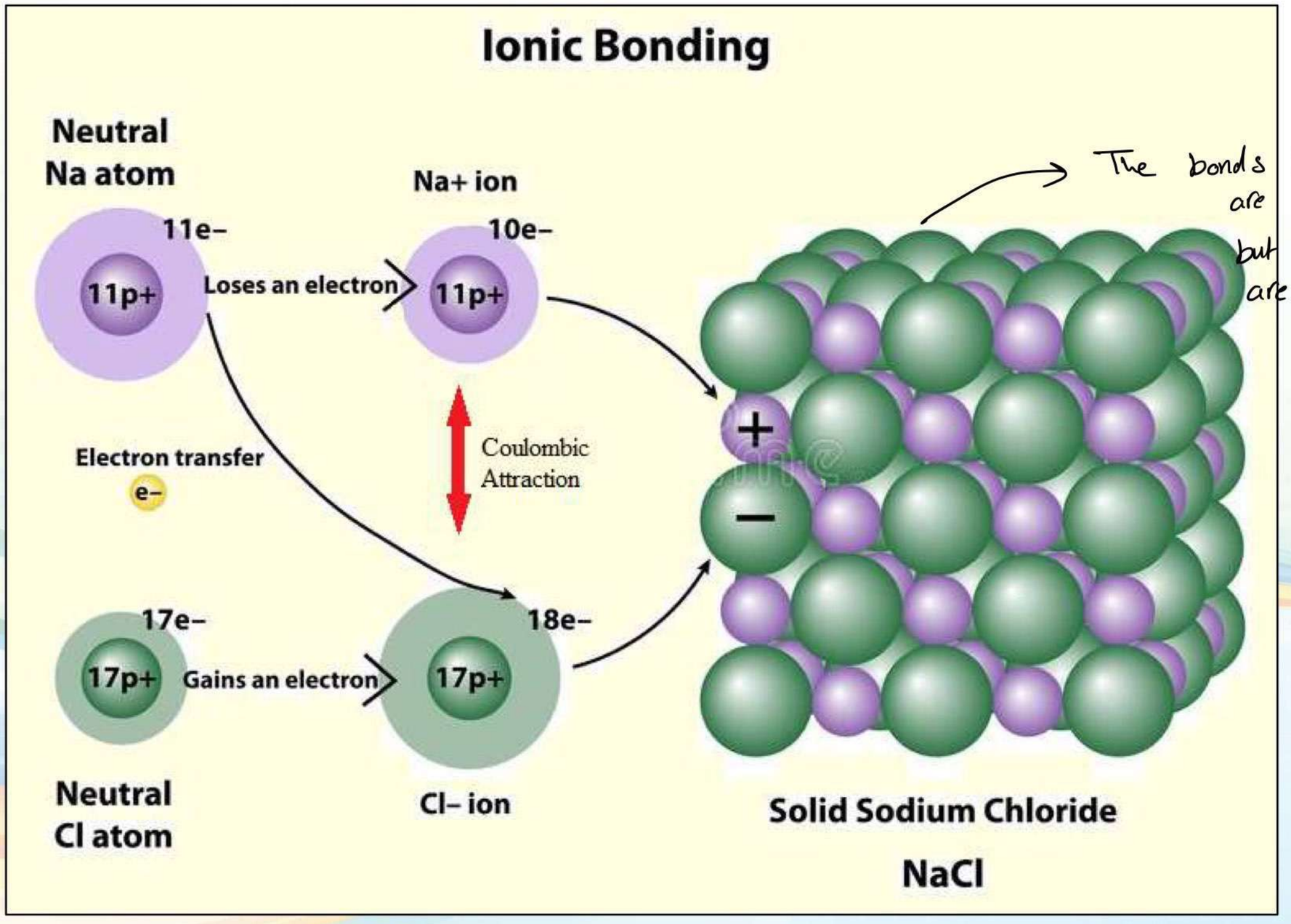
Formation of an Ionic Bond

⊛ There is a gap between two molecules due to repulsive force " the gap will increase if the repulsive force are high between them " (low electronegativity)

⊛ what is the minimum distance between Na and cl atom in NaCl ?

ans The radius of the Na ⊕ The radius of the cl

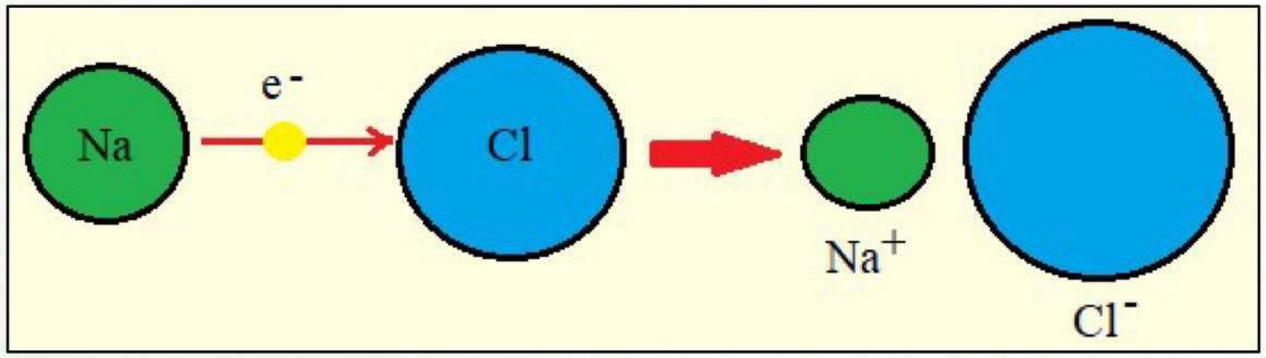
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The bonds between molecules are the secondary but between the atoms are ionic bonds

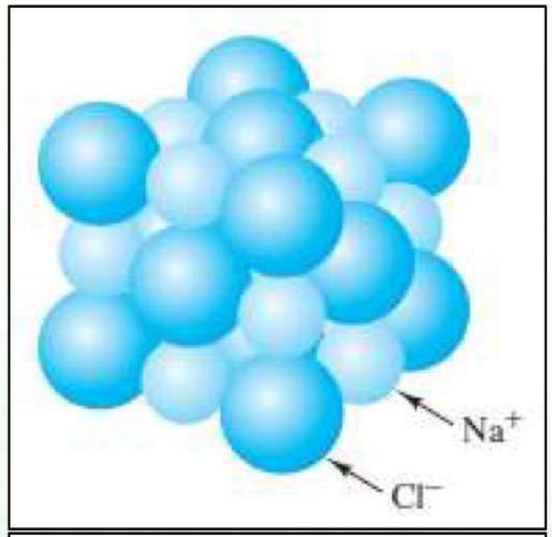
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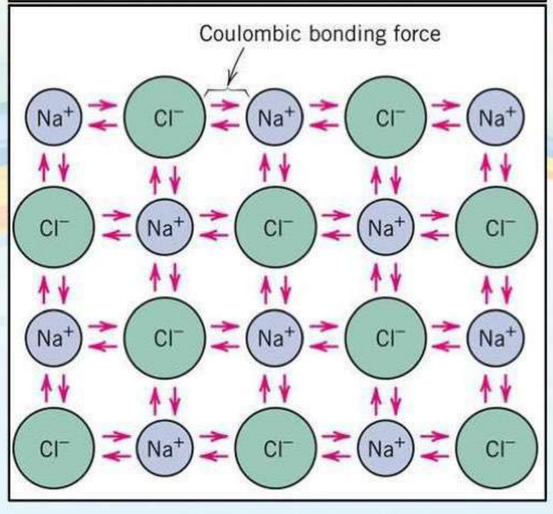
Ionic Bonding



→ all elements want to achive the minimum energy " => this energy is in the smallest distance between center to center

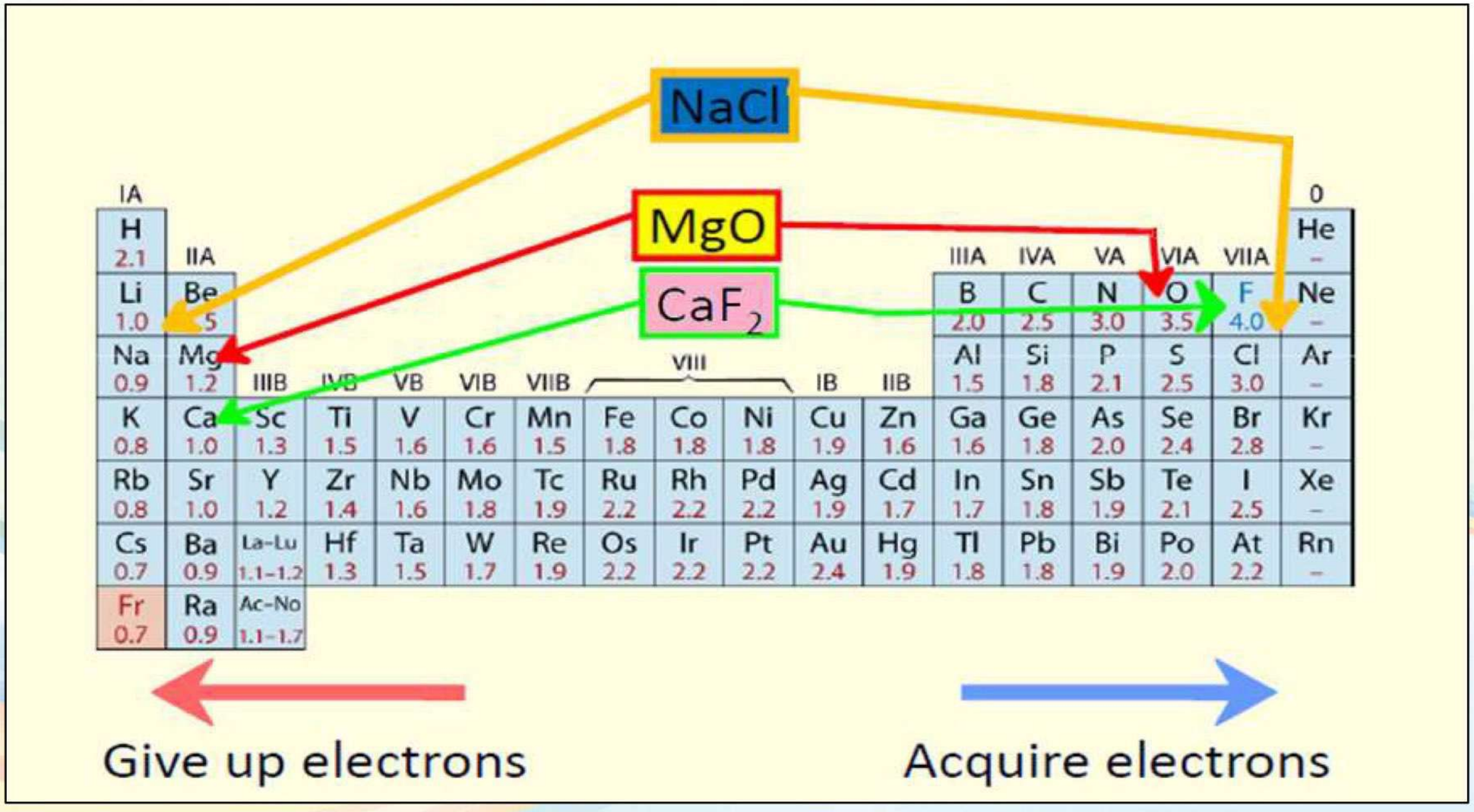
- ✓ *Electron transfer reduces the energy of the system of atoms, that is, electron transfer is energetically favorable.*
- ✓ *Note relative sizes of ions: Na shrinks and Cl expands*





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Ionic Bonding

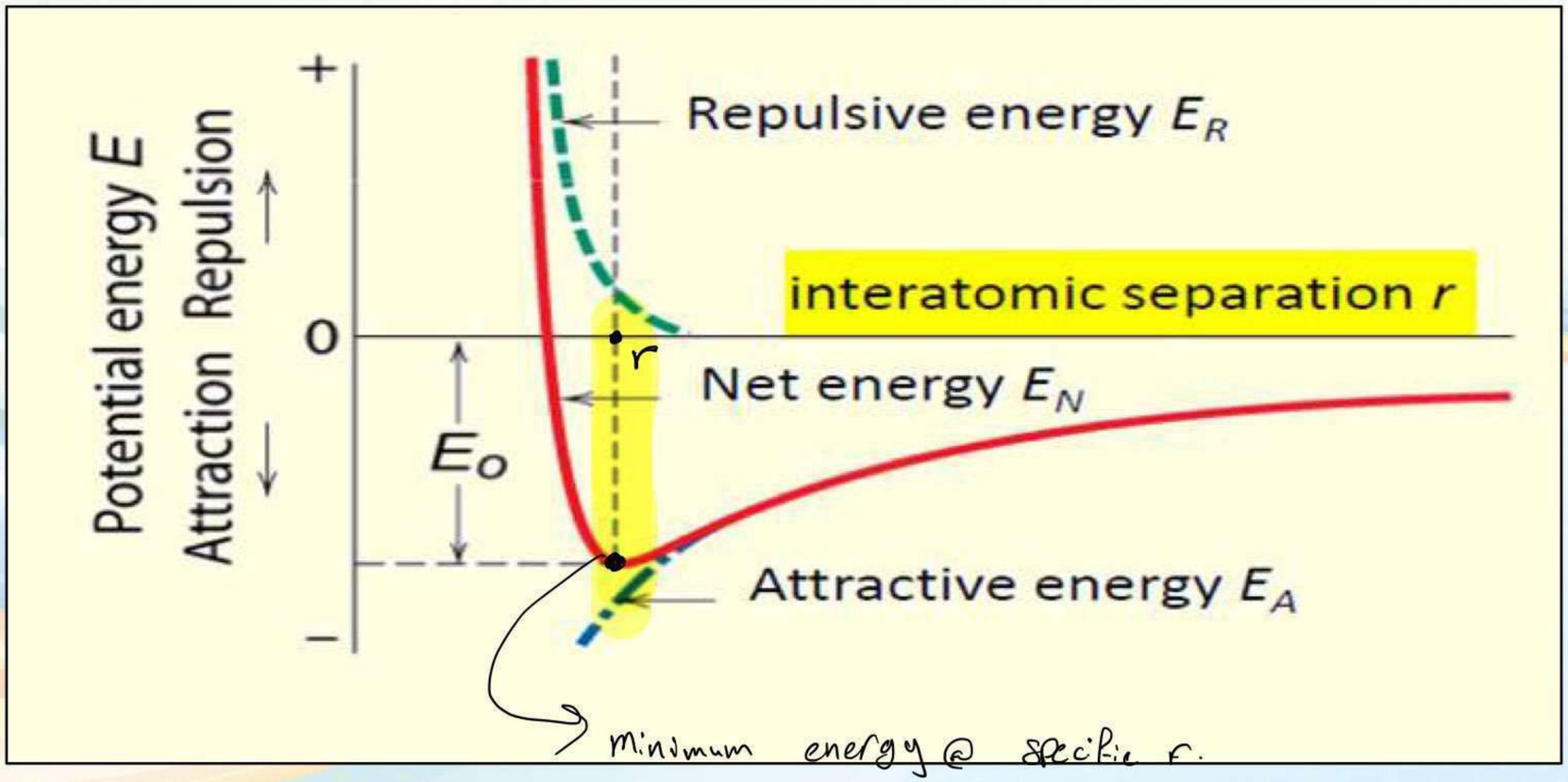


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Potential Energy

- In order for molecules to exist in aggregates in gases, liquids, or solids, there must be forces that attract the molecules together.

$$E_N = E_A + E_R$$



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(*) الـ [potential energy] مستحيل تساوي صفر.. ليش؟

لأنه لو كانت صفر فعلًا كانه رح يصير في تلاحس بين الذرتين

لهيك في بالنواة protons عشانه تخلقه قوى التنافر بين الذرتين والحفاظ على المسافة بين بعض

Potential Energy

- When the repulsive and attractive forces are equal the potential net energy is at a minimum and the system is stable.

Repulsive Forces

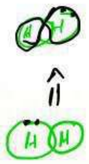
- The force is repulsive when the molecules are brought close enough together that the outer charge clouds of the molecules touch, and this causes the molecules to repel each other.
- The repulsive forces are necessary so that the molecules do not destroy each other

Attractive Forces

- The forces that bring molecules together are called forces of attraction.

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- They are mostly exsist as Liquid and gases because the molecules have more freedom to move within the substance
- low melting and Boiling points



انه عندي + صفات اما بكون فيها الكترونات الاخيرة

Covalent Bonding ⇒ there are a temporary Loss

(*) in ionic bonding they are non-directional not like covelent directional ⇒ they cannot change because its between the atom not the molecules.

- A covalent bond is formed when electrons are shared between atoms.
- Covalent bonds are between non-metals and non-metals or hydrogen and non-metals. ⇒ أو عنصر مع حالته زي H
- They share electrons so that both of them can have a stable octet.
- Covalent bonds are HIGHLY directional bonds.
- There are two types of covalent bonds:
  1. Non-polar: result when two exact non-metals equally share electrons. ⇐ O_2, H_2, N_2 —
  2. Polar: result when two different non-metals share electrons.

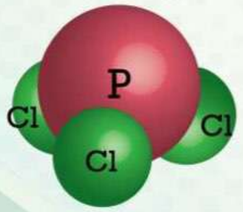
Such as H_2O, HNO_3 —

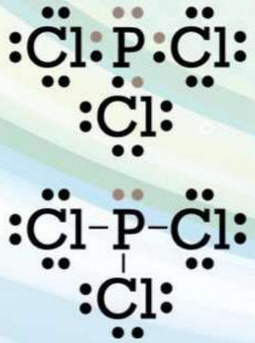
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Covalent Bonding

Phosphorus Trichloride

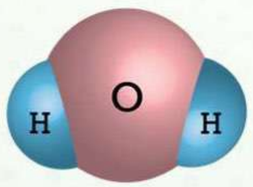
PCl_3

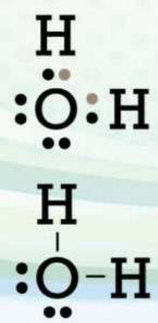




Water

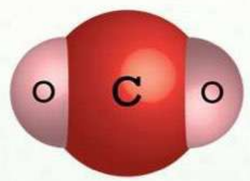
H_2O

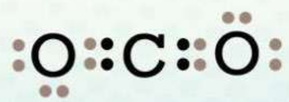


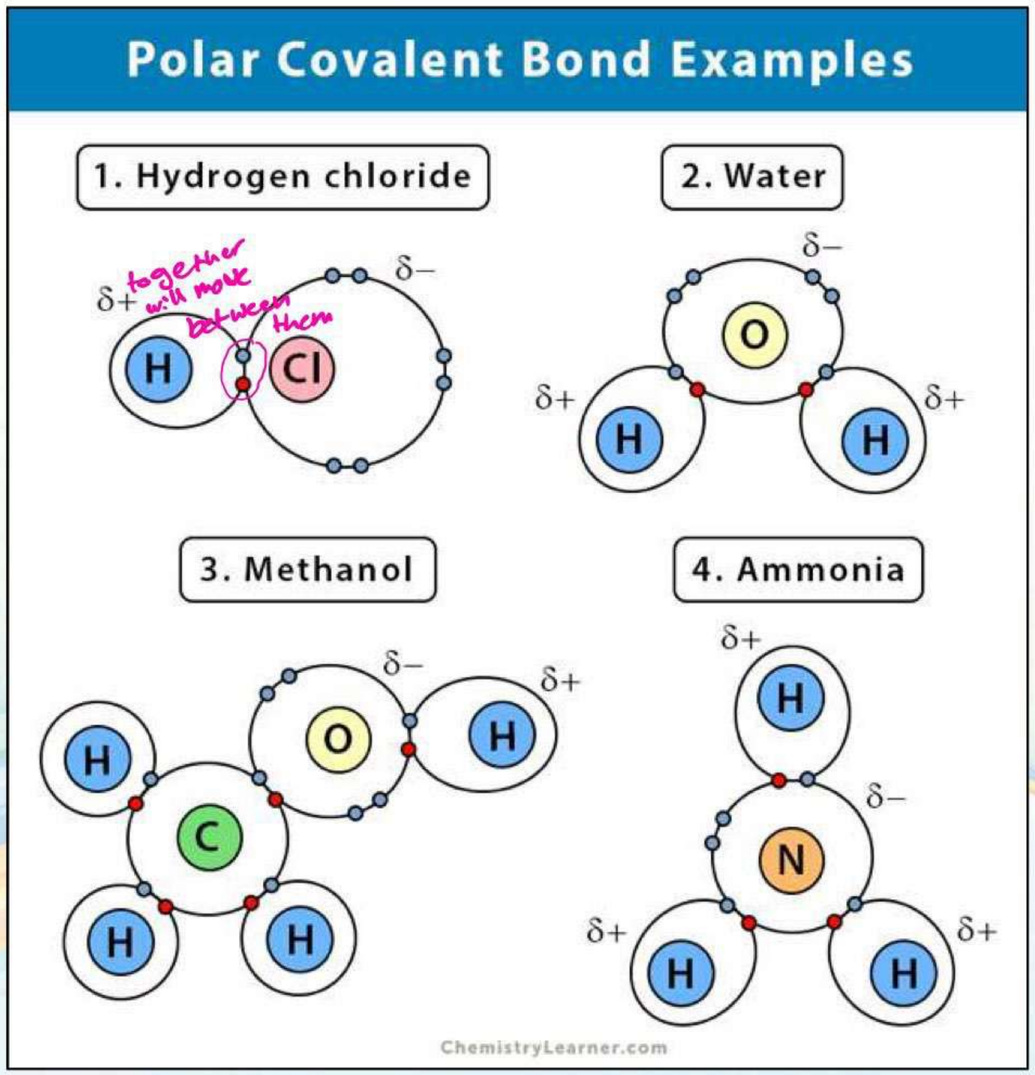


Carbon Dioxide

CO_2





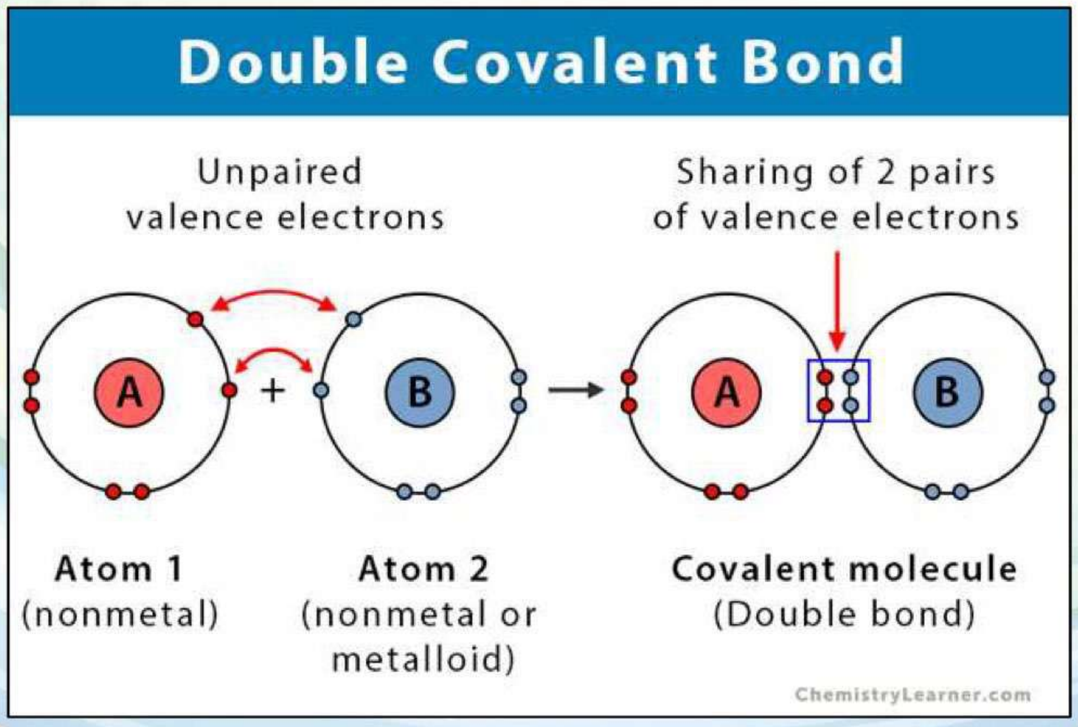


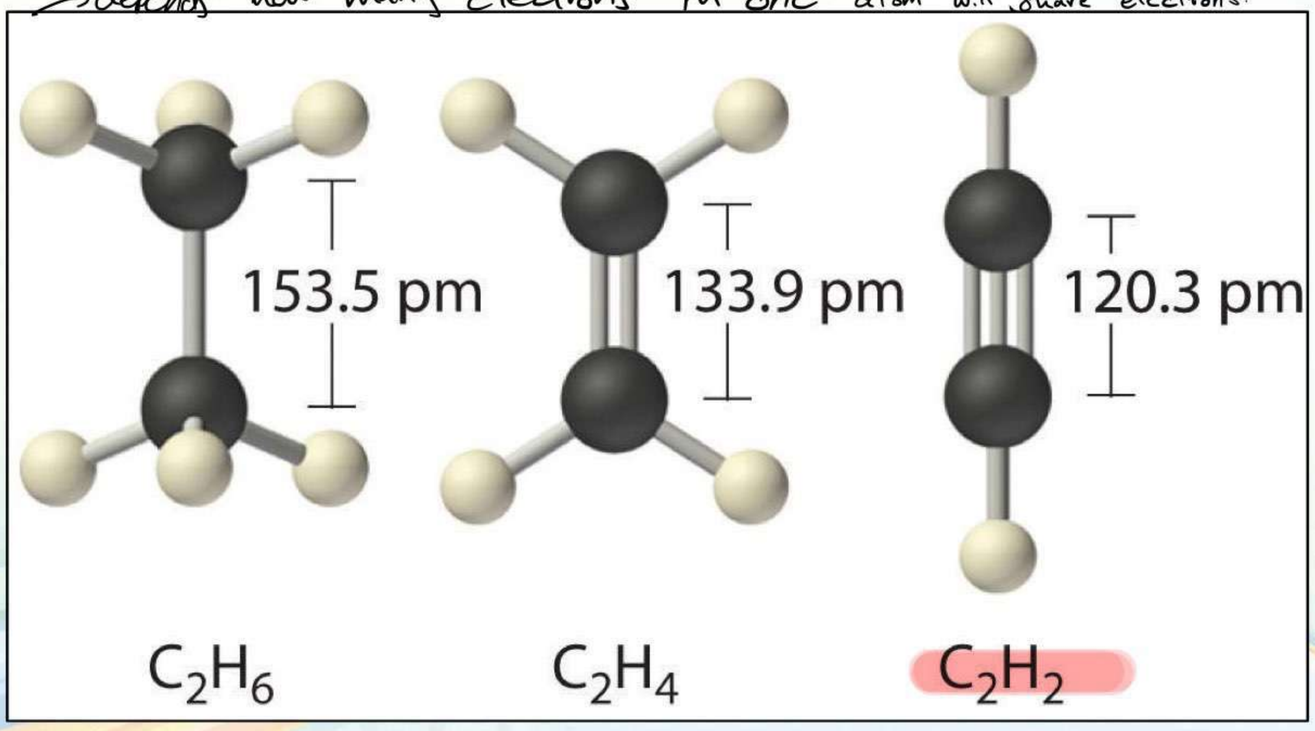
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Covalent Bonding

على أي أساس بنتخل الروابط ؟

depends how many electrons in one atom will share electrons.





$H - C \equiv C - H$

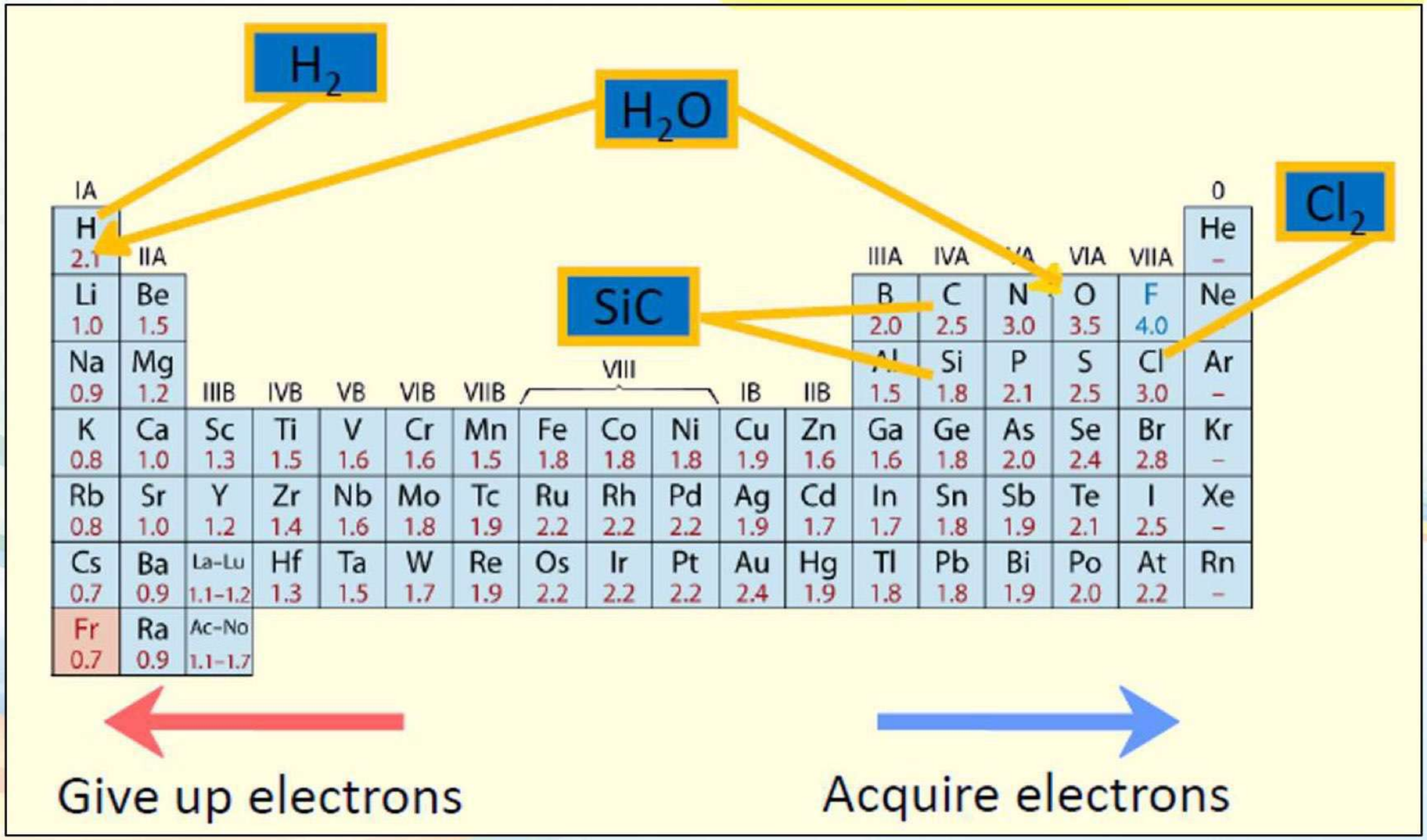
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(*) Acids are covelent Bonds => They are in Liquid state @ room tempreture

(*) Smelting => melting the metal
dissolution => ionization the metal.

Examples of Covalent Bonding

most of covelent compounds are weak.



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Naming Covalent Compounds

- Covalent compounds are much easier to name than ionic compounds; Examples:
  - ✓ P_2O_5 - diphosphorus pentoxide
  - ✓ CO - carbon monoxide
  - ✓ CF_4 - carbon tetrafluoride
- Some important exceptions to this naming scheme occur, examples:
  - ✓ H_2O is "water"
  - ✓ NH_3 is "ammonia"
  - ✓ CH_4 is "methane"

No of atoms	Prefix
1	Mono-
2	Di-
3	Tri-
4	Tetra-
5	Penta-
6	Hexa-
7	Hepta-

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What are the properties of covalent compounds

- Covalent compounds generally have much lower melting and boiling points than ionic compounds.
- Covalent compounds are soft and squishy (compared to ionic compounds).
- Covalent compounds tend to be more flammable than ionic compounds.
- Covalent compounds don't conduct electricity in water. (because the electrons are the responsible to move the currents here, they are not free to move "directional")
- Like dissolves like. This means that compounds tend to dissolve in other compounds that have similar properties (particularly polarity). (depends on it)
- Since water is a polar solvent and most covalent compounds are fairly nonpolar.

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- good conductor of electricity
- ductility
- thermal and electrical conductivity + resistivity

not directional bonds

Metallic Bonds

we consider each element is an anion.

* generally metals are ions.

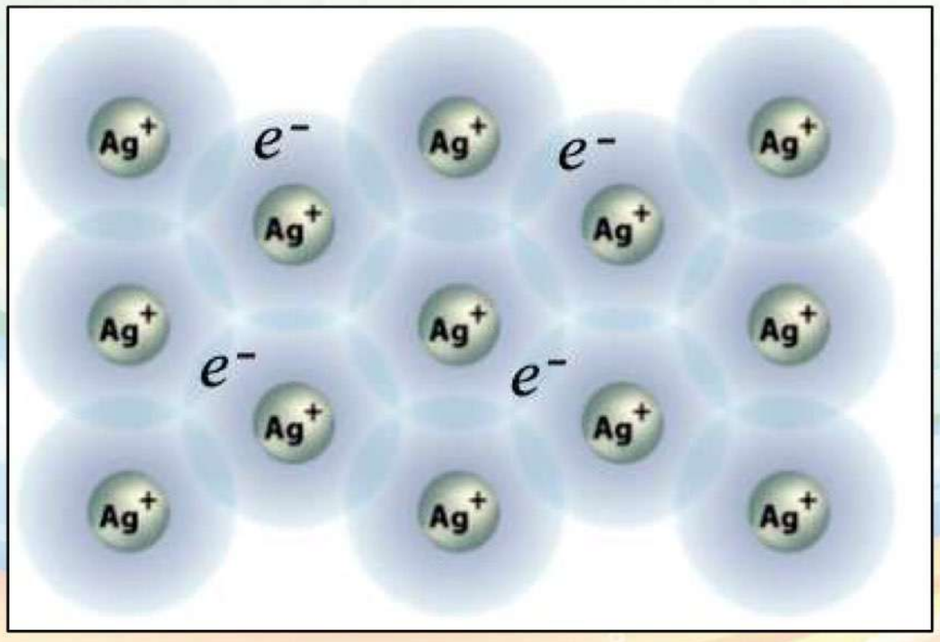
- *Metallic bonding occurs in metallic substances.*
- *Atoms of metals are held together in this structure by the sharing effect of the electrons amongst all of the atoms.*
- *This forms a "sea" or a "cloud" of free electrons that floats around the surface of metals.*
- *The crystal lattice of metals consists of ions NOT atoms surrounded by a 'sea of electrons' forming another type of giant lattice.*

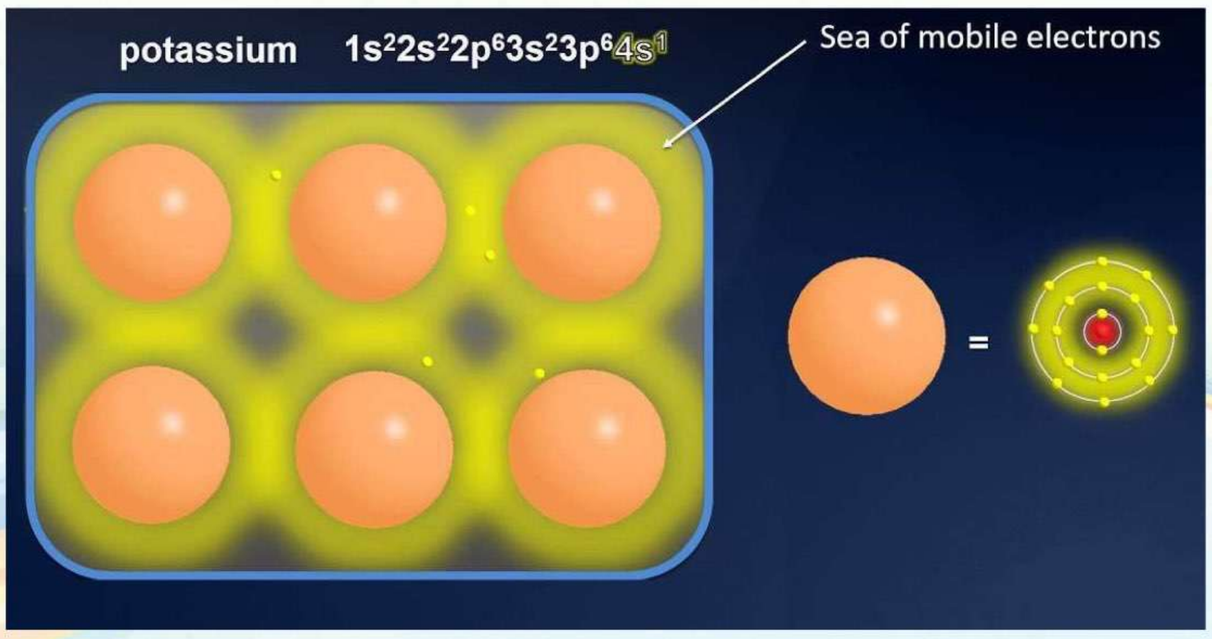
covalent are metallic

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Metallic Bonds

- A metallic bond is non-directional (bonds form in any direction) → atoms pack closely





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* Hg ⇒ has a metallic bonding but it's weak.

Properties of Metallic Bonds

- The strong bonding generally results in dense, strong materials with high melting and boiling points.
- Metals are good conductors of electricity because these 'free' electrons carry the charge of an electric current when a potential difference (voltage) is applied across a piece of metal.
- Metals are also good conductors of heat. This is also due to the free moving electrons.
- Typical metals also have a silvery surface, but remember this may be easily tarnished by corrosive oxidation in air and water.

(otherwise it's not silvery because of it's reactivity)

- Unlike ionic solids, metals are very malleable, they can be readily bent, pressed or hammered into shape. The layers of atoms can slide over each other without fracturing the structure . The reason for this is the mobility of the electrons

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(+) Fe_3C ⇒ between Fe and C are metalic bonding but between Fe_3C and Fe_3C are secondary bonding

The secondary bond is weak relative to the primary within the

mainly between molecule and noble gases.

Secondary bonding - Intermolecular Forces ⇒ تتشكل بسبب السكتات في الجزيئات

- Secondary, Van der Waals, or physical bonds are weak in comparison to the primary bonds.
- Secondary bonding exists between virtually all atoms or molecules, but its presence may be obscured if any of the three primary bonding types is present.
- Secondary bonding forces arise from atomic or molecular dipoles.
- An electric dipole exists whenever there is some separation of positive and negative portions of an atom or molecule.
- The bonding results from the Coulombic attraction between the positive end of one dipole and the negative region of an adjacent one
- Dipole interactions occur between:
  1- Fluctuated (تذبذب) induced dipoles.
  2- Permanent (دائم) dipole bond.
  3- Polar molecule-induced dipole

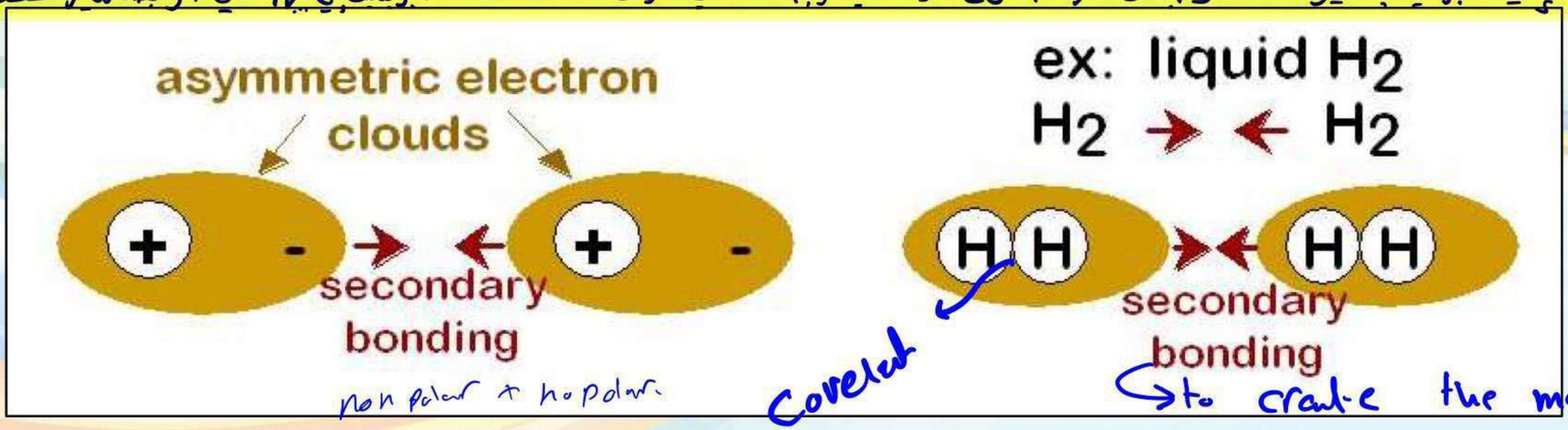
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(non polar + non polar) between 2 similar atoms.

Fluctuating induced dipoles

- Very weak electric dipole bonding can take place among atoms due to an instantaneous asymmetrical distribution of electron densities around their nuclei.
- This type of bonding is termed fluctuation since the electron density is continuously changing.

في اللاحظة إلي الجزيء بتغير شحنته موجبة والتحز سالبة رح تتكون هاي الرابطة لكنه هي مؤقتة أدل ما حدث الجزيئ إلي بيهم هاي الرابطة تتغير شحنته رح تتفكك



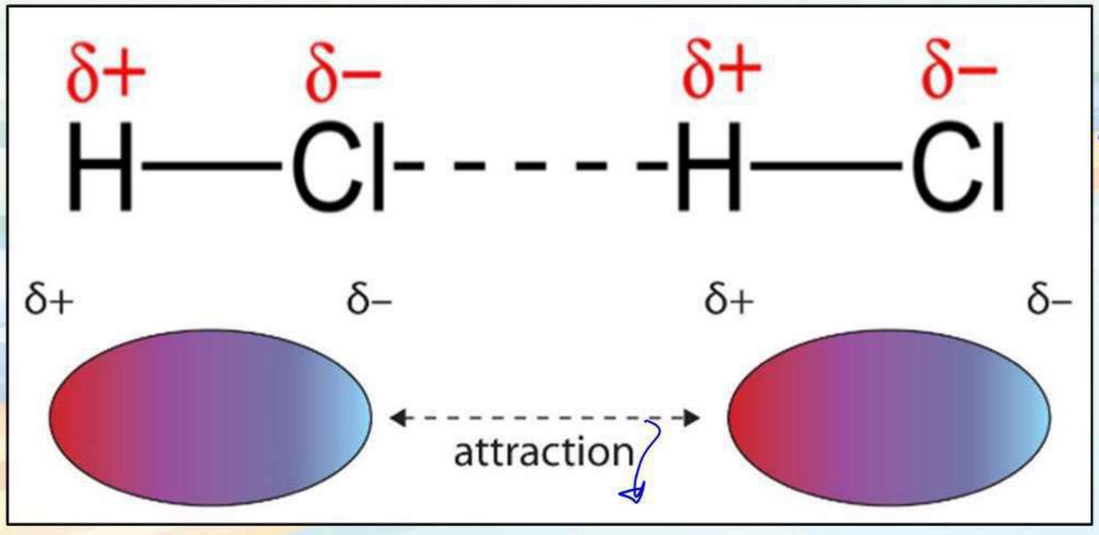
covelent

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Permanent dipoles ⇒ 2 molecule with dissimilar atoms.

→ polar + polar

- *Coulombic forces also exist between adjacent polar molecules.*
- *Weak intermolecular bonds are formed between molecules which possess permanent dipoles.*
- *A dipole exists in a molecule if there is asymmetry in its electron density distribution.*



This bond is fixed

هاي الرابطة تكوّنت بين ذرتين H-Cl هاي
وبين اللي تكوّنت بين H من جزيء
covelent bonding
H-Cl و Cl من جزيء آخر H-Cl هاي
وهي أكيد أضعف من covelent
permanent
لهيك ما إنفصل H. من H-Cl و Cl من H-Cl الثاني.

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1) non + non => fluctuated

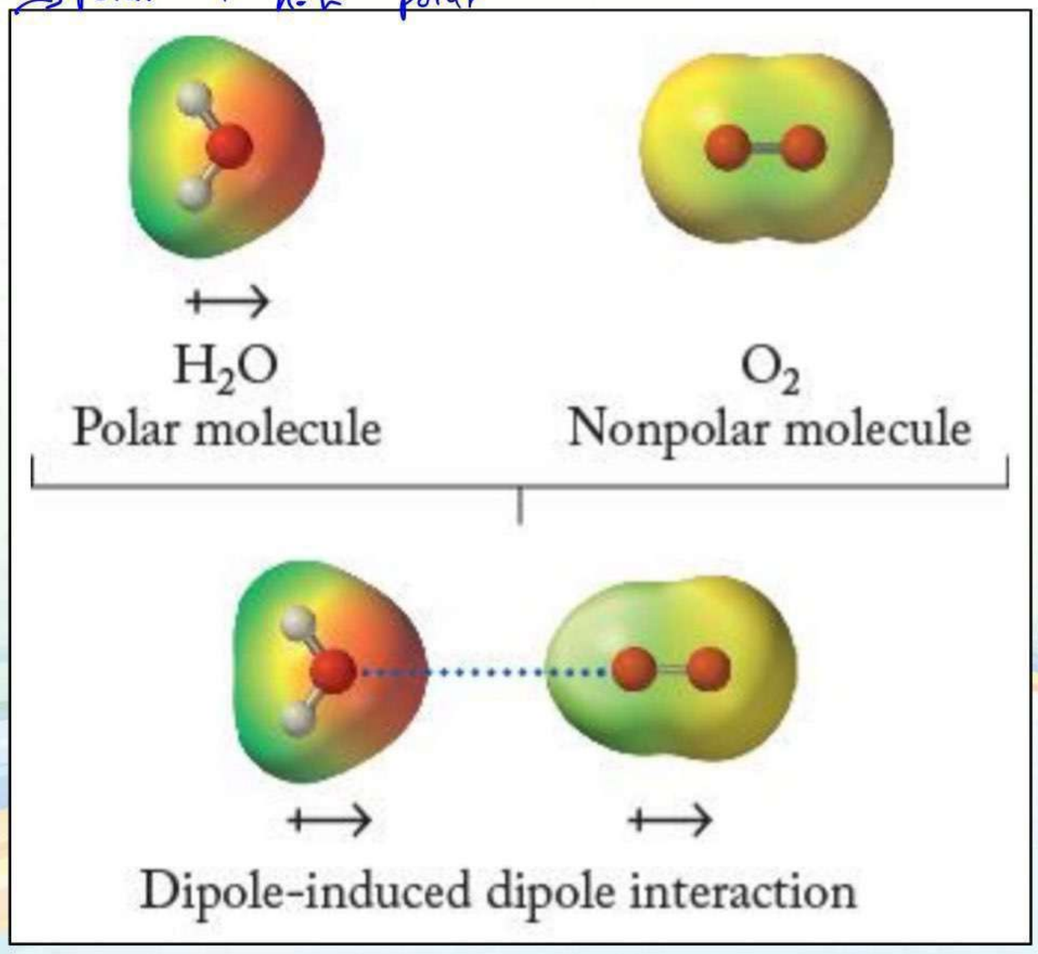
2) polar + polar => permanent

3) polar + non => polar molecule induced.

Polar molecules - induced dipole

- Polar molecules (with asymmetric arrangement of positively and negatively charged regions) can induce dipoles in adjacent nonpolar molecules

→ Polar + non polar



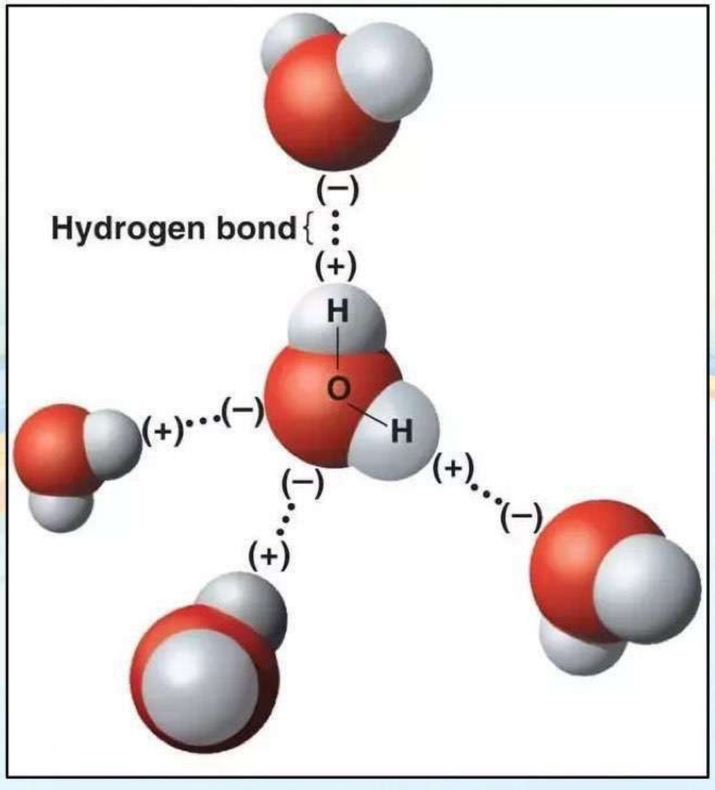
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Hydrogen bonding

- Hydrogen bonding, a special type of secondary bonding, is found to exist between some molecules that have hydrogen as one of the constituents.
- An intermolecular attraction between a partially positively charged hydrogen in one molecule and a partially negatively charged oxygen, nitrogen, or fluorine in a nearby molecule

Example:

Hydrogen bond in water. The H end of the molecule is positively charged and can bond to the negative side of another H2O molecule (the O side of the H2O dipole)



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Type	Bond Energy	Comments
Ionic	Large	Nondirectional (ceramics)
Covalent strong in solid structure	Variable Large-Diamond Small-Bismuth	Directional (semiconductors, ceramics, polymer chains)
Metallic	Variable Large-Tungsten Small-Mercury	Nondirectional (metals)
Secondary	Smallest	Directional Inter-chain (polymer) Inter-molecular

fluctuated => directional for a moment but also a non directional when the charge of one molecule changes

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Bonding and materials properties

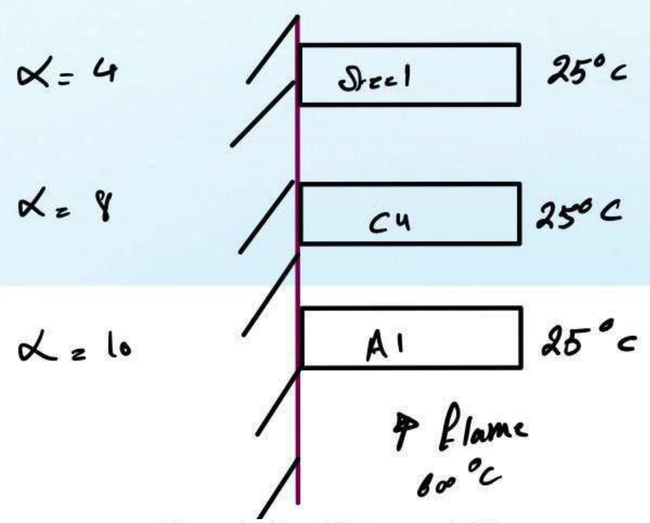
- Materials with large bonding energies usually have high melting temperatures.
- There is a correlation between the magnitude of the bonding energy and the state of materials
  - ✓ Solids have large bonding energies
  - ✓ Liquids tend to have relatively lower energies

Bonding energy ↑ so we expect the state of the material to have a solid state.

- The expansion/contraction during heating/cooling of materials is related to the shape of its E(r) curve.

All metals have a contraction and expansion coefficients 'function of T'

- A deep and narrow 'trough,' which typically occurs for materials having large bonding energies, usually imply a low coefficient of thermal expansion.

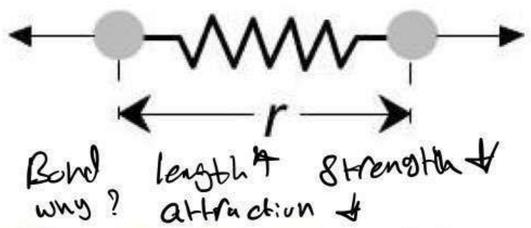


Al will expa
than Cu Ha
Steel
ΔL = α ΔT

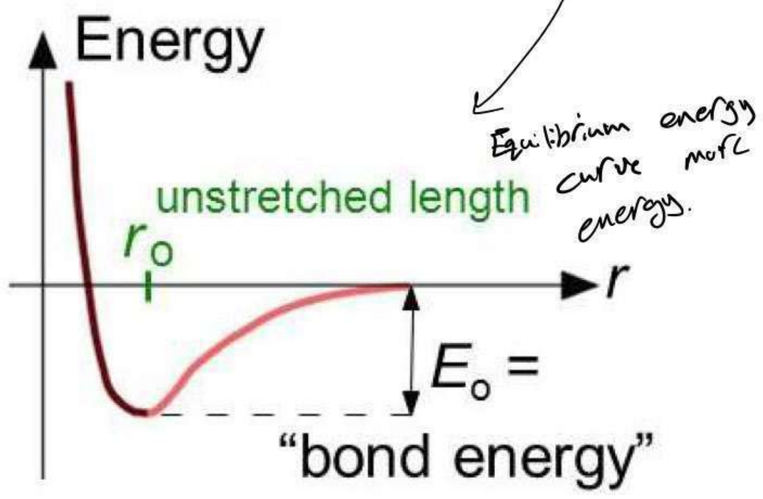
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Properties From Bonding: T_m

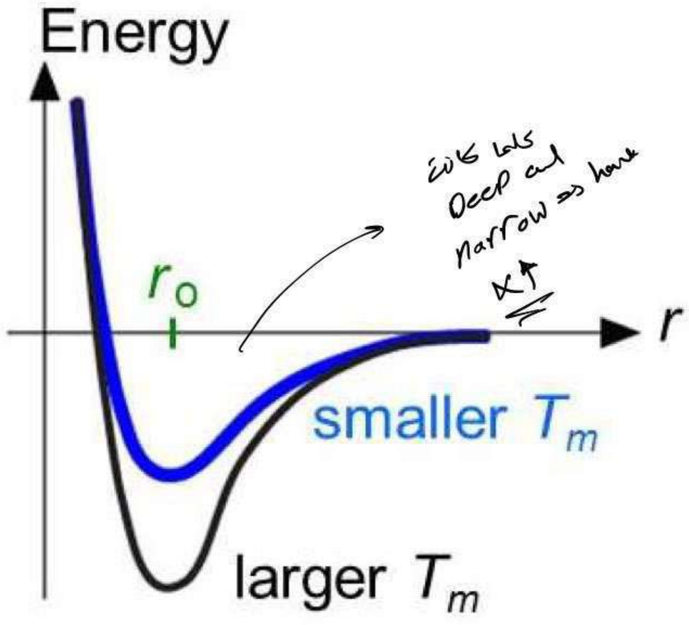
- Bond length, r



- Bond energy, E_o



- Melting Temperature, T_m



T_m is larger if E_o is larger.

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Chapter 3

The Structure of Crystalline Solids Part A

The University of Jordan
Chemical Engineering Department
First Semester 2021
Prof. Yousef Mubarak

adar
ask & believe & recieve

⊛ All metals are in crystal structure

⊛ in polycrystalline structure

example on single crystal structure

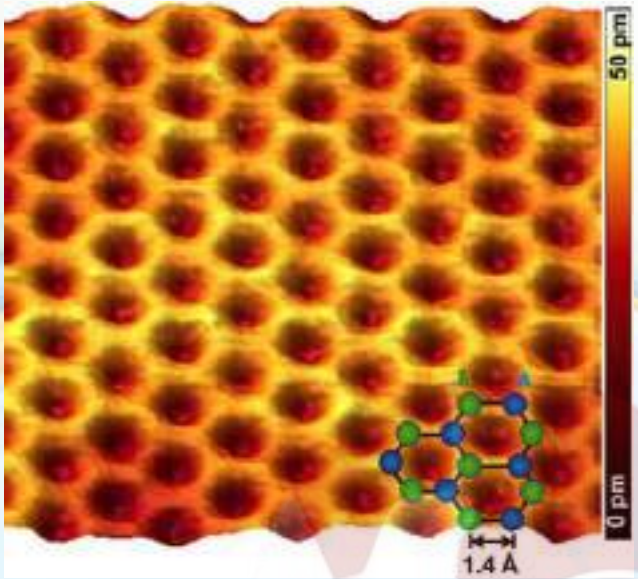
1) diamond

2) NaCl



→ Single crystal





⊛ كلما كانت الزرة داخل البلورة منظم أكثر كلما كانت البلورة أصح شكل

وهذا هو الفرق الرئيسي بينها وبين Amorphous structure

Outline

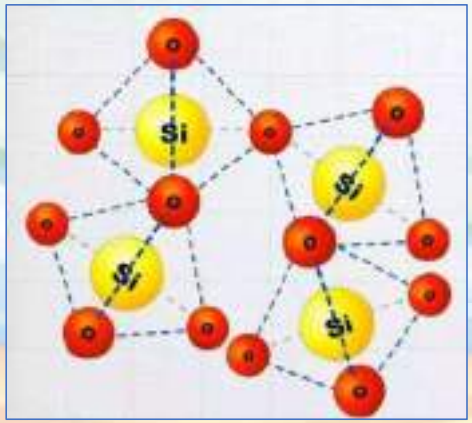
- How do atoms arrange themselves to form solids?
- Types of solids
  1. Single crystal
  2. Polycrystalline
  3. Amorphous
- Fundamental concepts
- Unit cells
- Crystal structures
  1. Simple cubic
  2. Face-centered cubic
  3. Body-centered cubic
  4. Hexagonal close-packed
- Close packed crystal structures
- Density computations

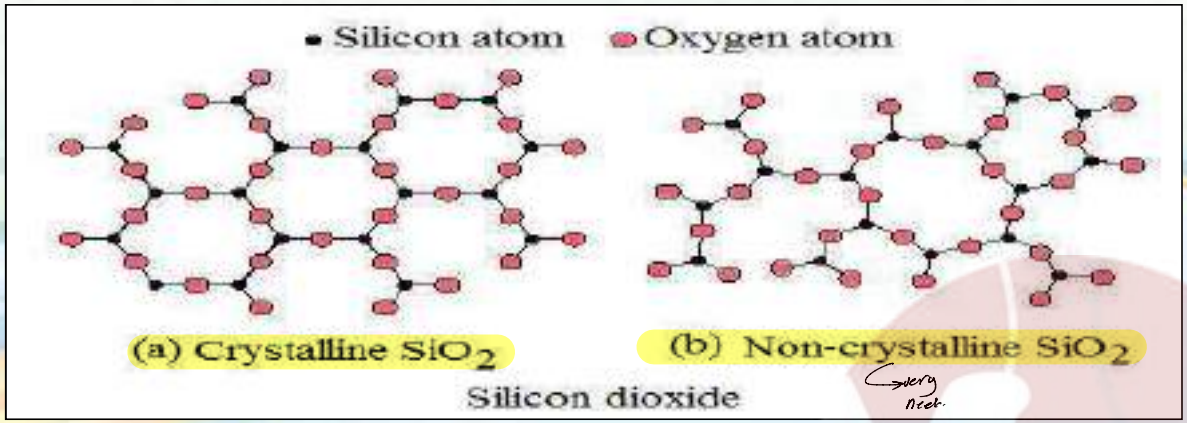
ask & believe & recieve

We can convert crystals ⇒ amorphous

Types of solids

- **Crystalline material:** atoms self-organize in a periodic array:
  1. Single crystal: atoms are in a repeating or periodic array over the entire extent of the material → such as diamonds.
  2. Polycrystalline material: comprised of many small crystals or grains ⇒ crystallites very small
- **Amorphous:** lacks a systematic atomic arrangement

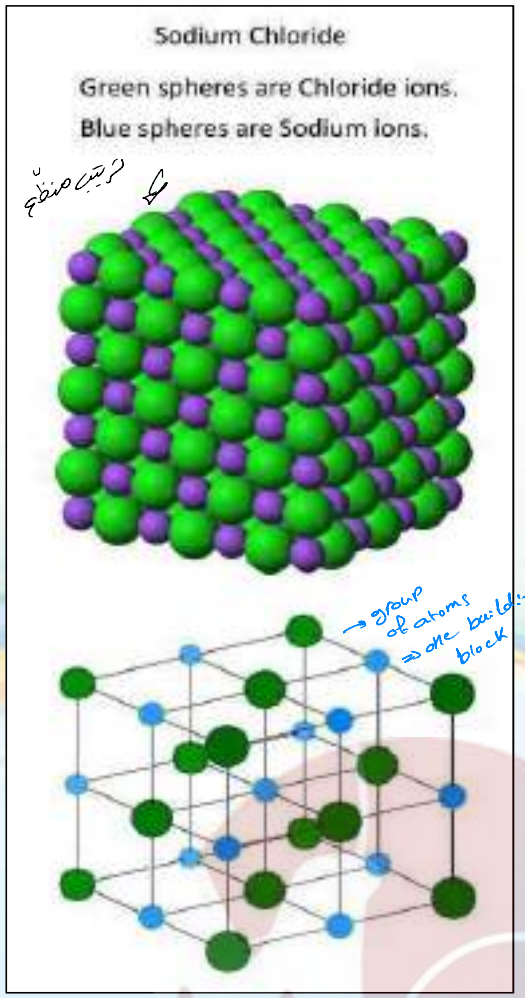




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Crystal Structure

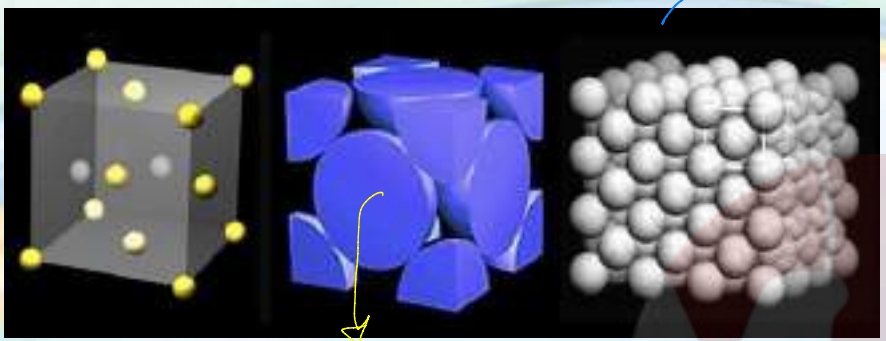
- To discuss crystalline structures it is useful to consider atoms as being hard spheres with well-defined radii.
- In this hard-sphere model, the shortest distance between two like atoms is one diameter.
- We can also consider crystalline structure as a lattice of points at atom/sphere centers.



Unit Cell

- The unit cell is the smallest structural unit or building block that can describe the crystal structure. ⇒ it's not the smallest structure in the material.
- Repetition of the unit cell generates the entire crystal.
- Example: 2D honeycomb net can be represented by translation of two adjacent atoms that form a unit cell for this 2D crystalline structure.





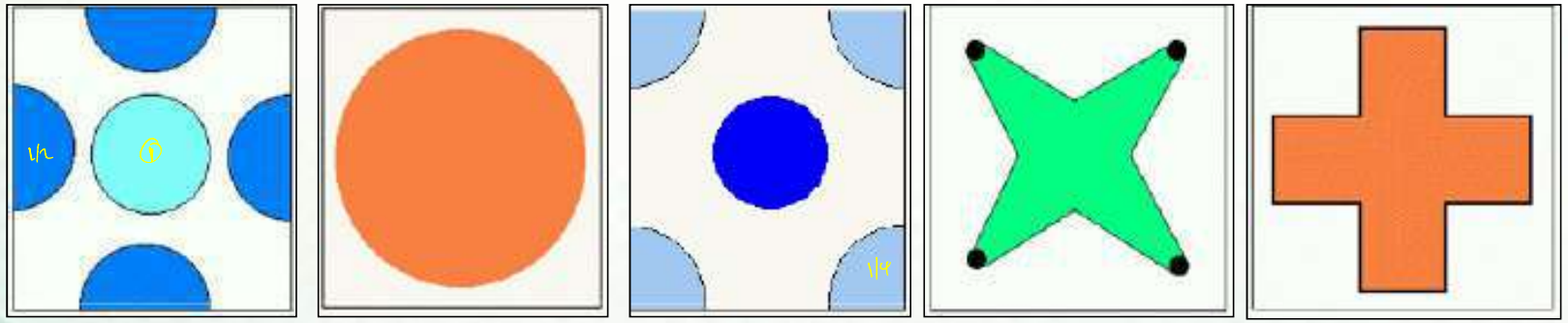
Example of 3D crystalline structure:

when will one atom contribute (*) in 100% in one building block?

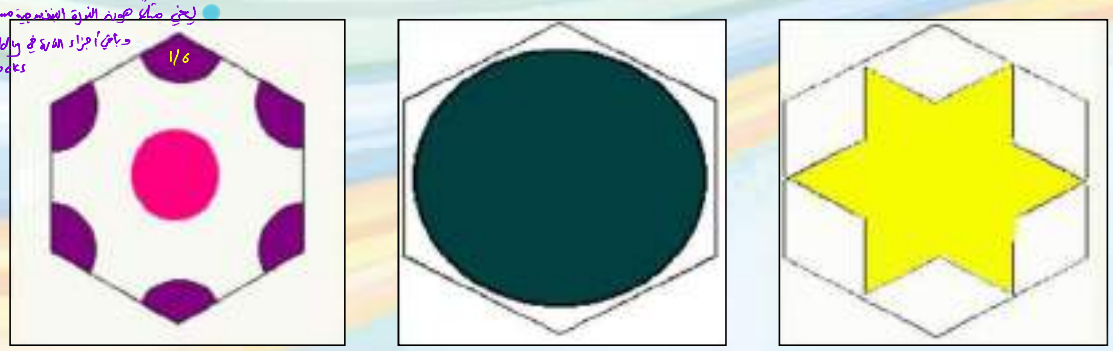
Ans when we put the atom (one sphere) in the center of building block

- *Different choices of unit cells are possible, for example:*

  A square unit cell may contain any of the following object patterns.



- *One hexagonal unit cell might look like any of the following.*

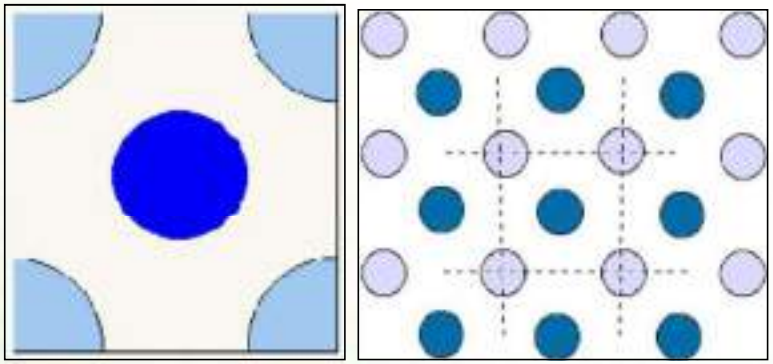


Crystalline Lattices

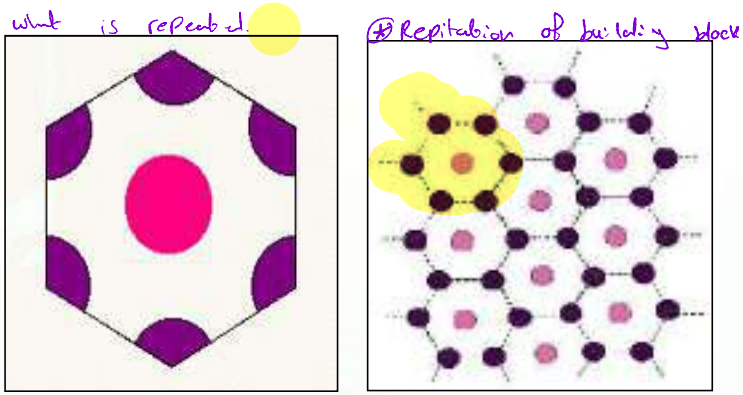
- A crystal is a repeating array. In describing this structure we must distinguish between the pattern of repetition (the lattice type) and what is repeated (the unit cell).
- The most fundamental property of a crystal lattice is its symmetry. If we initially limit ourselves to 2 dimensions for simplicity, three types are present:

1. Squares
2. Rectangles
3. Hexagons

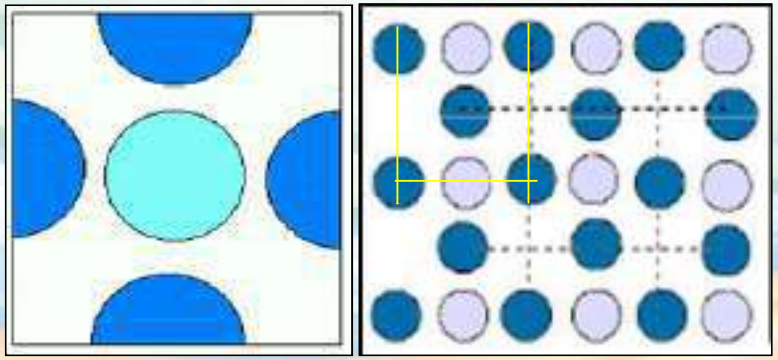
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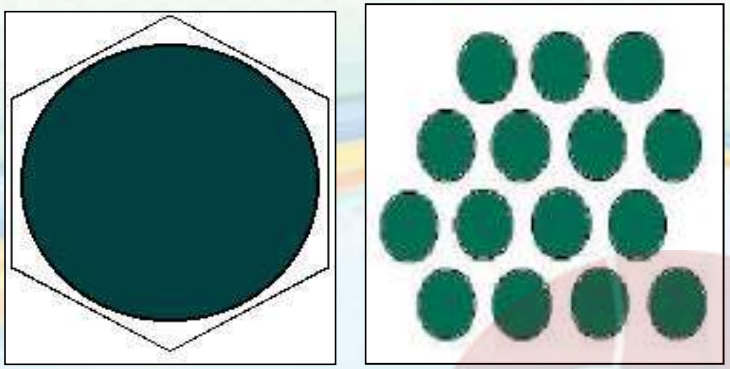
unit cell lattice



unit cell lattice



unit cell lattice



unit cell lattice

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Metallic Crystal Structures

=> to describe the structure in a very accurate way we have to represent it in the three dimensions.

- Metals tend to be densely packed.
- Reasons for dense packing:
  - Typically, only one element is present, so all atomic radii are the same.
- Metals tend to be densely packed.
  - Metallic bonding is not directional.
  - Nearest neighbor distances tend to be small in order to lower bond energy.
- Have the simplest crystal structures.

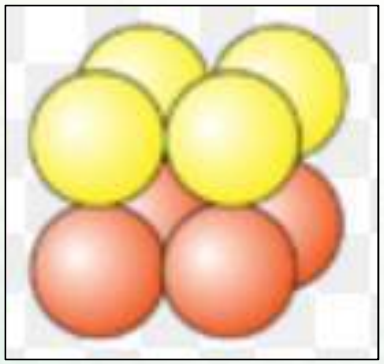
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- Metals are usually (poly)crystalline.
- Although formation of amorphous metals is possible by rapid cooling. ⇒ عشانه مش بيسمح للذرات تترتب على شكل كريستال
- The atomic bonding in metals is non-directional ⇒ no restriction on numbers or positions of nearest-neighbor atoms ⇒ large number of nearest neighbors and dense atomic packing.
- Atom (hard sphere) radius, R, defined by ion core radius - typically 0.1 - 0.2 nm

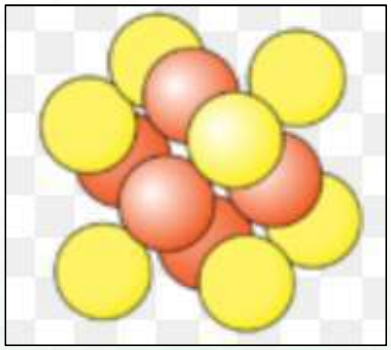
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The most common types of unit cells are:

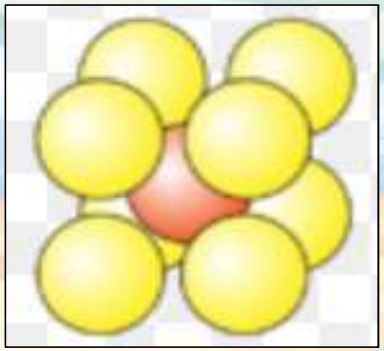
1- The simple cubic (SC)



2- The faced centered cubic (FCC).



3- The body-centered cubic (BCC)



4- The hexagonal close-packed (HCP)

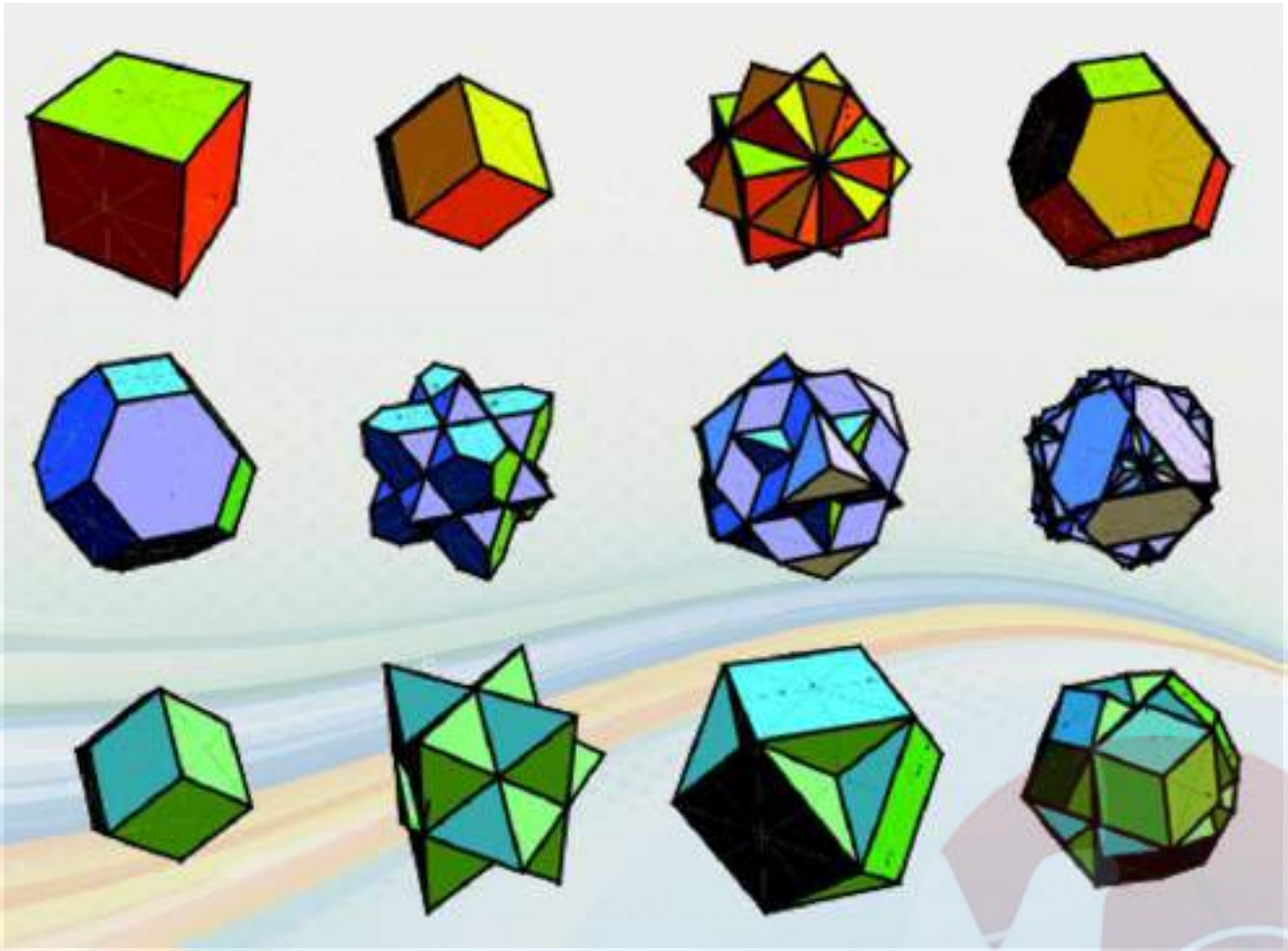


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Simple cubic

Faced centered cubic

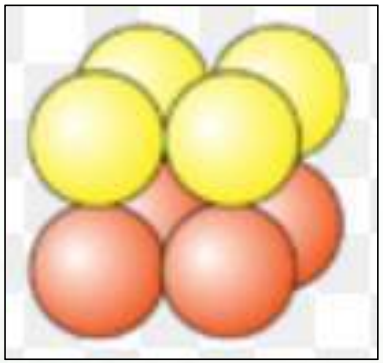
Body-centered cubic

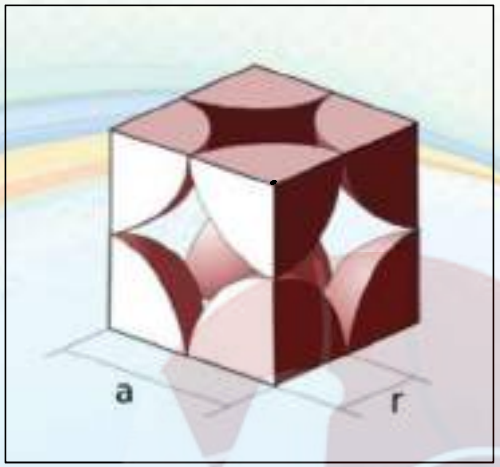


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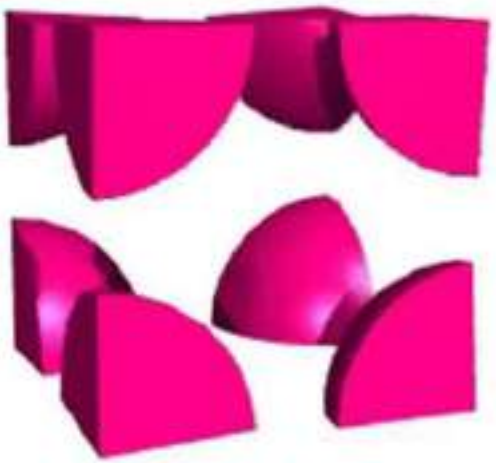
Simple Cubic Metal

- Rare due to low packing density.
  - Only Po has this structure.
  - Close-packed directions are cube edges.
- In a metal the atoms are all identical, and most are spherical (the bonding does not depend on direction). => if it's not identical the distribution of the packing eff will be hard.
- Metals thus tend to adopt relatively simple structures. The simplest is simple cubic.





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- Coordination number = 6 atoms (it's the maximum number of atoms that touches one atom directly.)
- Number of atoms per unit cell:

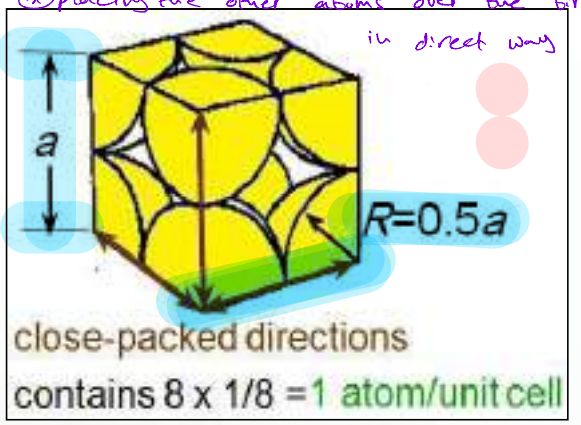
  = 8 corners x 1/8

  = 1 atoms

(it's very important to determine it to calculate packing effeciency.)

arranging of atoms in simple cube:-

① placing the other atoms over the first layer in direct way



- In 3-D the packing efficiency is given by :
  - ✓ P.E. = (Volume of spheres) / (volume of cell)
  - ✓ For a simple cubic lattice, this is:

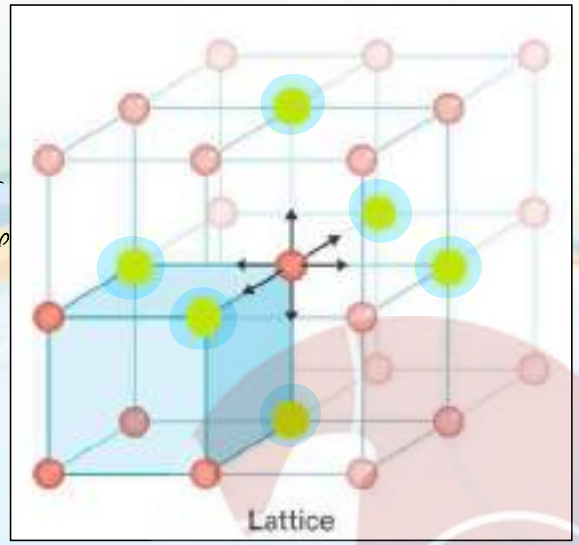
$$\text{Volume of spheres} = \frac{1}{8} \times 8 \times \frac{4}{3} \times \frac{22}{7} \times (0.5a)^3$$

(number of atoms; we have to know what is the relationship between a and r)

$$\text{Volume of cell} = (a)^3 \Rightarrow a = 2R = 8r^3$$

(volume of cube)

$$\therefore P.E. = \frac{88}{168} = 0.523$$

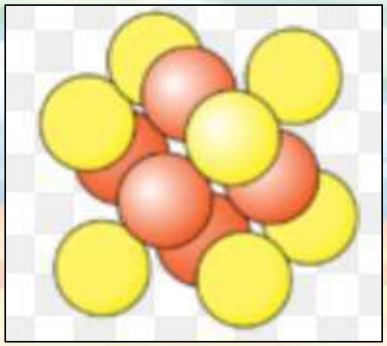
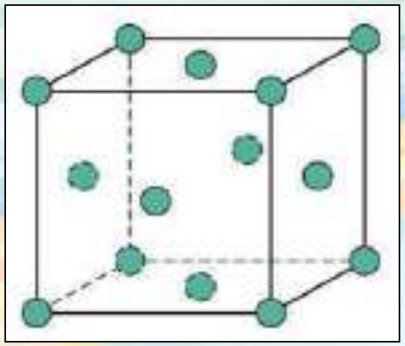
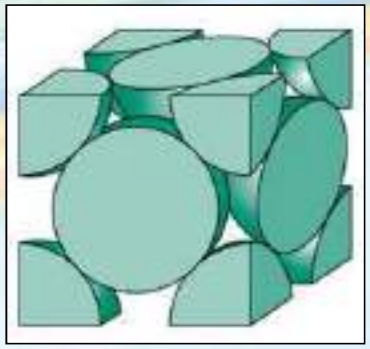
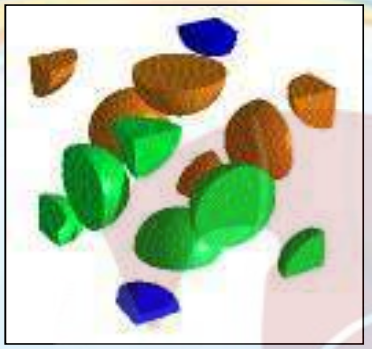


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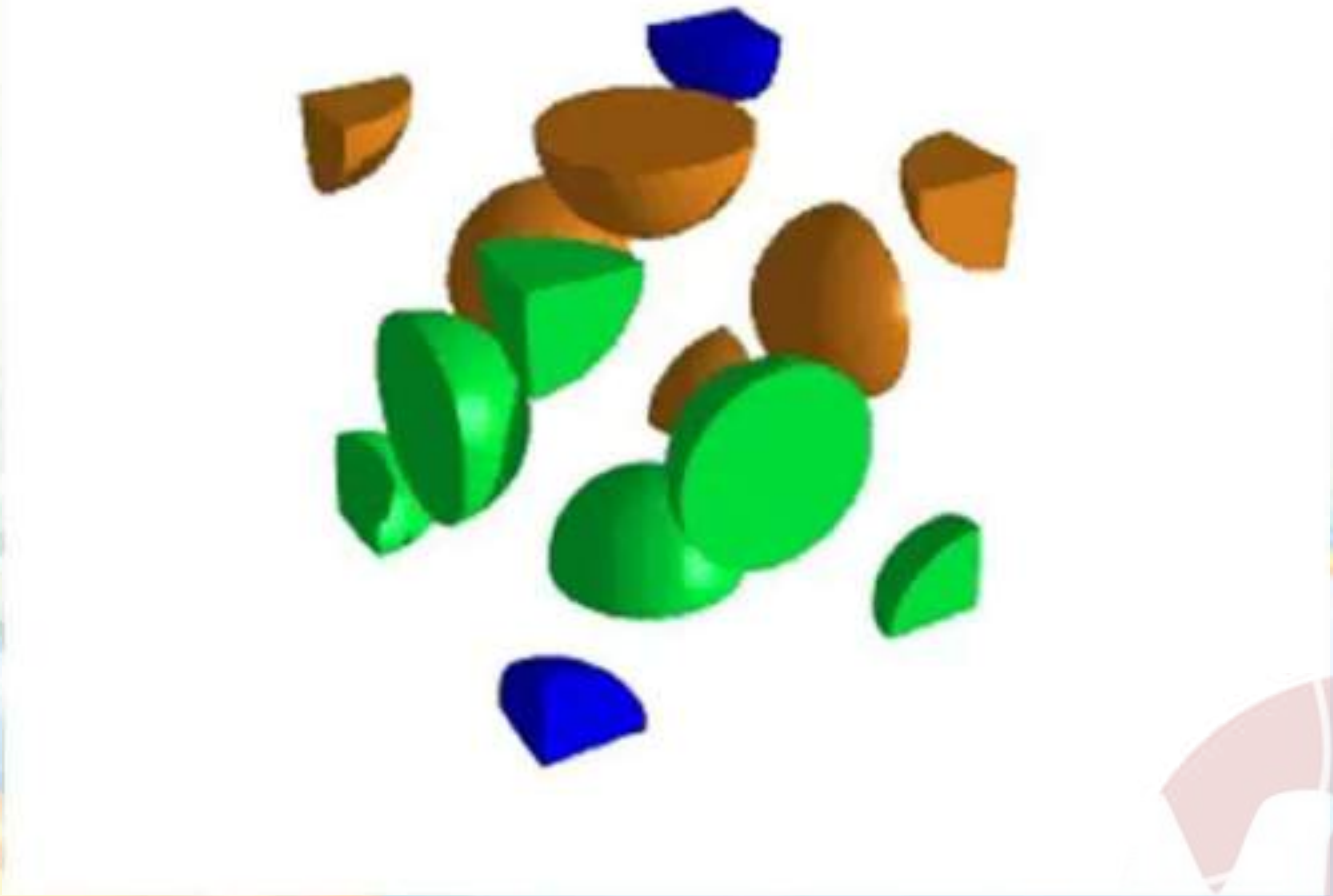
Face Centered Cubic (FCC)
or
Cubic Close Packed (CCP)

⇒ any compounds has covelent or ionic bonding have these types of arrangents.

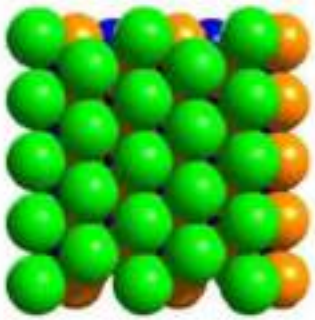
- Think of this cell as being made by inserting another atom into each face of the simple cubic lattice - hence the "face centered cubic" name .
- The reason for the various colors is to help point out how the cells stack in the solid .

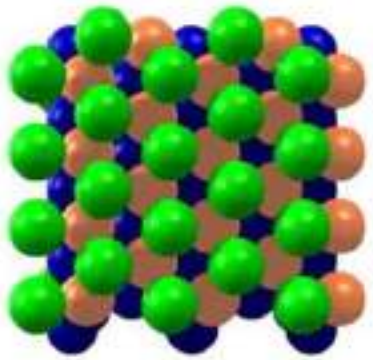





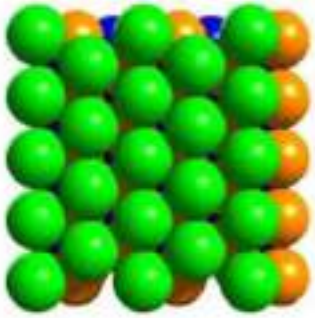
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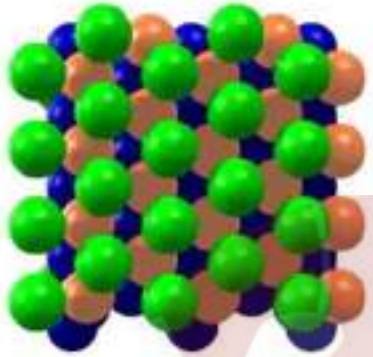


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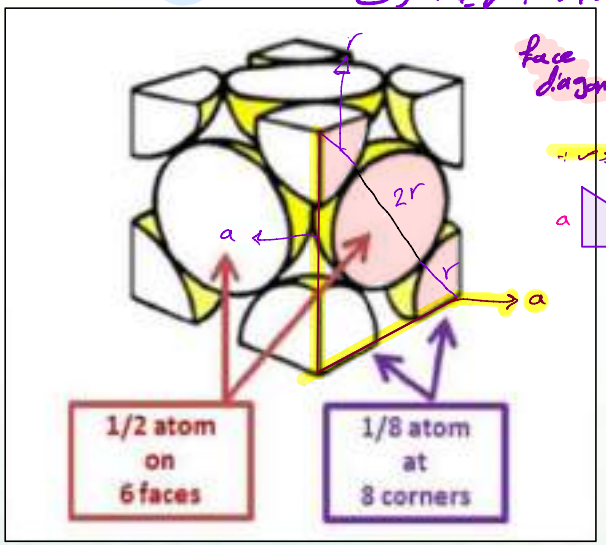
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- Atoms touch each other along face diagonals.
  - ✓ Note: All atoms are identical.
- Example:
  - ✓ Al, Cu, Au, Pb, Ni, Pt, Ag ⇒ al Alkaline mebals also.
- Coordination number = 12 atoms ⇒ Maximum coordinbion number exsict in mebals = 12 !!
- Number of atoms per unit cell:

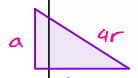
= 6 face x 1/2 + 8 corners x 1/8 = 4



لبس السؤال هاي بتوعلاقة ٩٠ مع ٤٥
بلزم أدوّل على انهاد مباشرية الذرات
وهو بقع في ال face diagonal



عن طريقة نظرية فيثاغورس ب

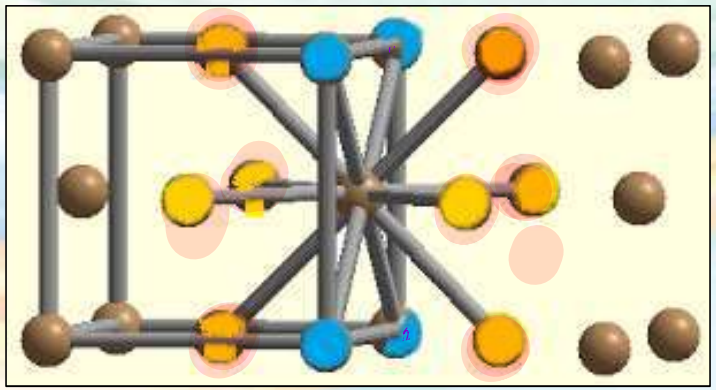


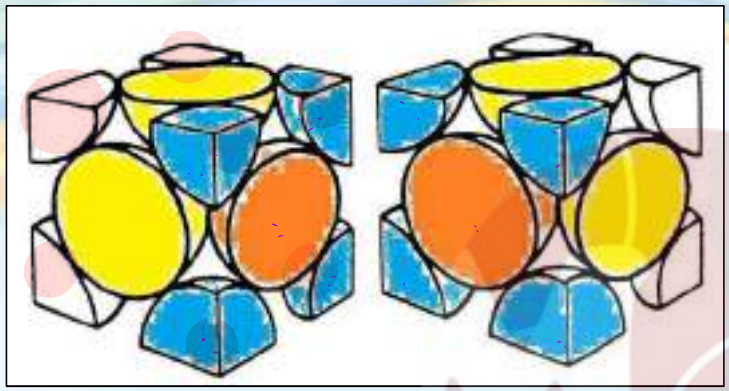
$16r^2 = a^2 + a^2$

$16r^2 = 2a^2$

$8r^2 = a^2$

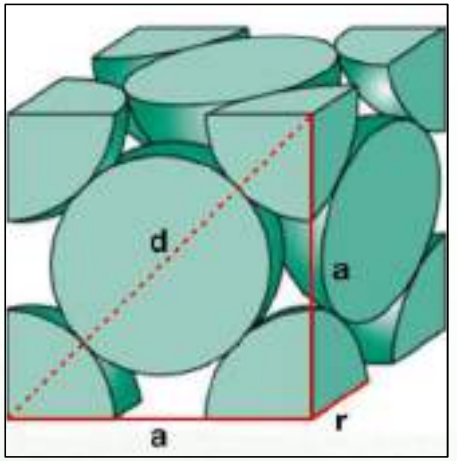
$a = \sqrt{8}\, r$

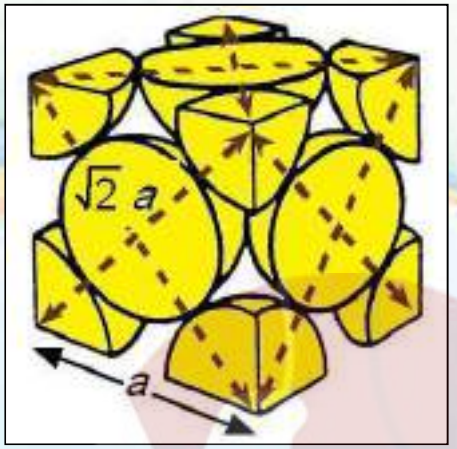




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- *In 3-D the packing efficiency is given by :*
  - ✓ *P.E. = (Volume of spheres) / (volume of cell)*
- *For a face centered cubic lattice, this is:*





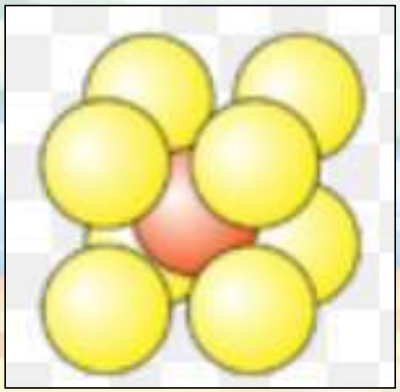
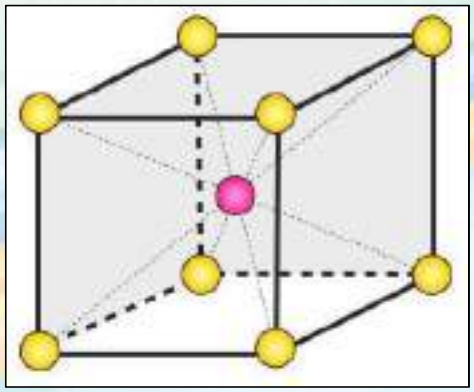
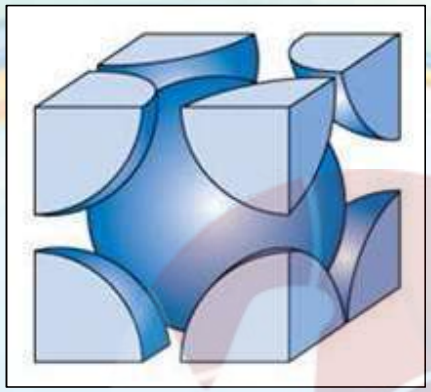
$$Volume\ of\ spheres = 4 \times \frac{4}{3} \times \frac{22}{7} \times \left(\frac{a\sqrt{2}}{4}\right)^3$$

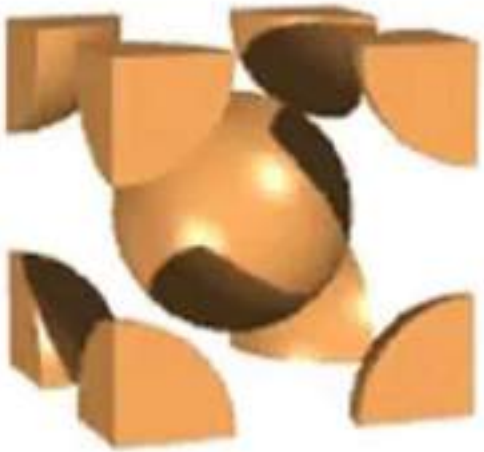
$$Volume\ of\ cell = (a)^3$$

$$\therefore P.E. = \frac{995.6}{1344} = 0.7405$$

Body Centered Cubic Structure (BCC)

- Think of this unit cell as made by stuffing another atom into the center of the simple cubic lattice, slightly spreading the corners.
- The corner spheres no longer quite touch one another, but do touch the center.
- Examples: Cr, W, Fe (α), Tantalum, Molybdenum





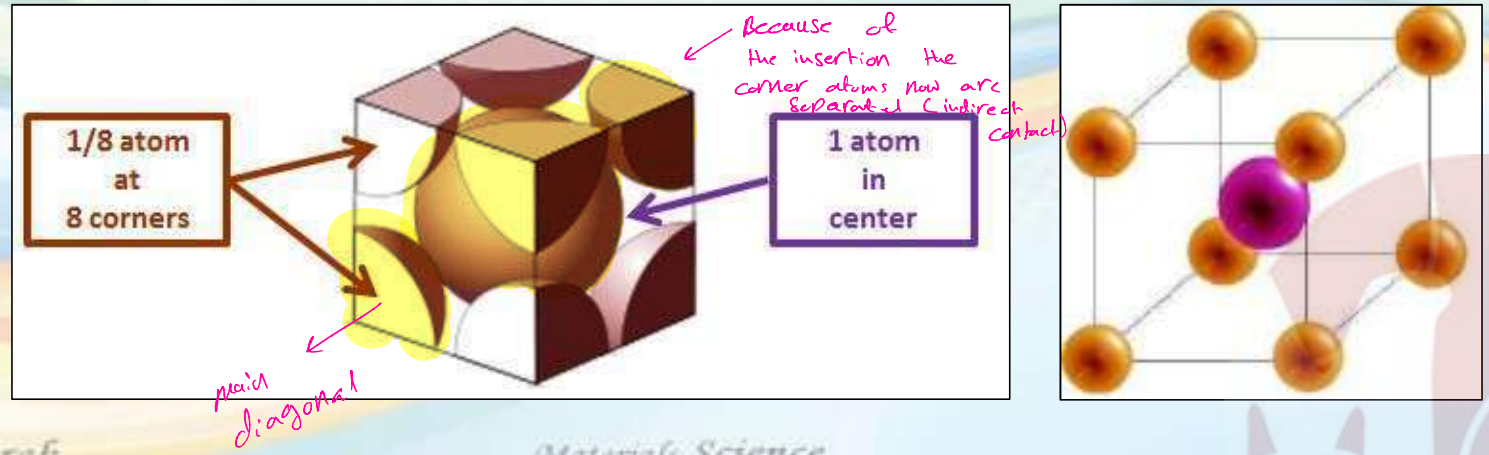
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- The hard spheres touch one another along cube diagonal
- The coordination number, CN = 8
- Number of atoms per unit cell, n = 2

  1 center atom shared by no other cells: 1 x 1 = 1

  8 corner atoms shared by eight cells: 8 x 1/8 = 1

- Corner and center atoms are equivalent



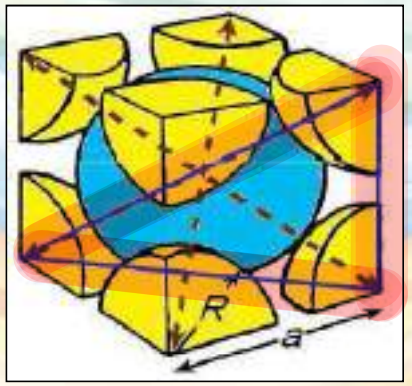
⇒ *the cube edge length, a= 4R/√3*

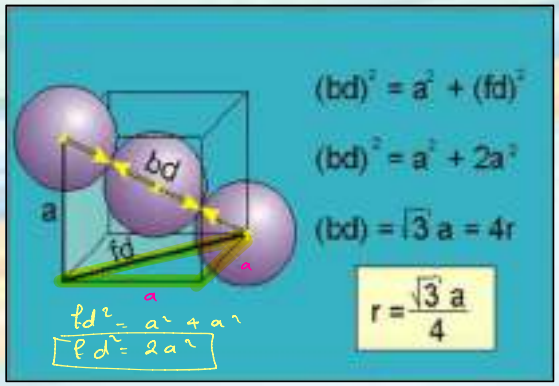
$$Volume\ of\ spheres = 2 \times \frac{4}{3} \times \frac{22}{7} \times \left(\frac{a\sqrt{3}}{4}\right)^3$$

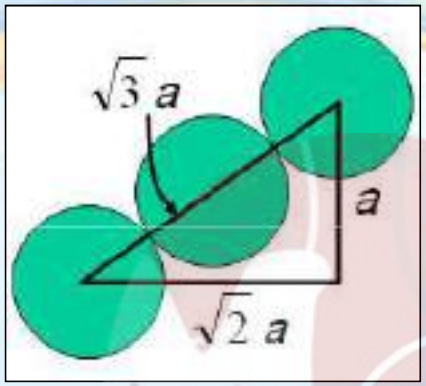
$$Volume\ of\ cell = (a)^3$$

$$\therefore P.E. = \frac{914.5}{1344} = 0.6805$$

- *The higher coordination number and packing efficiency mean that this lattice uses space more efficiently than simple cubic.*

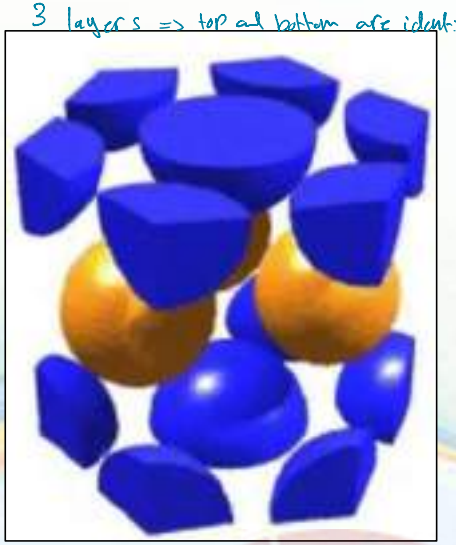




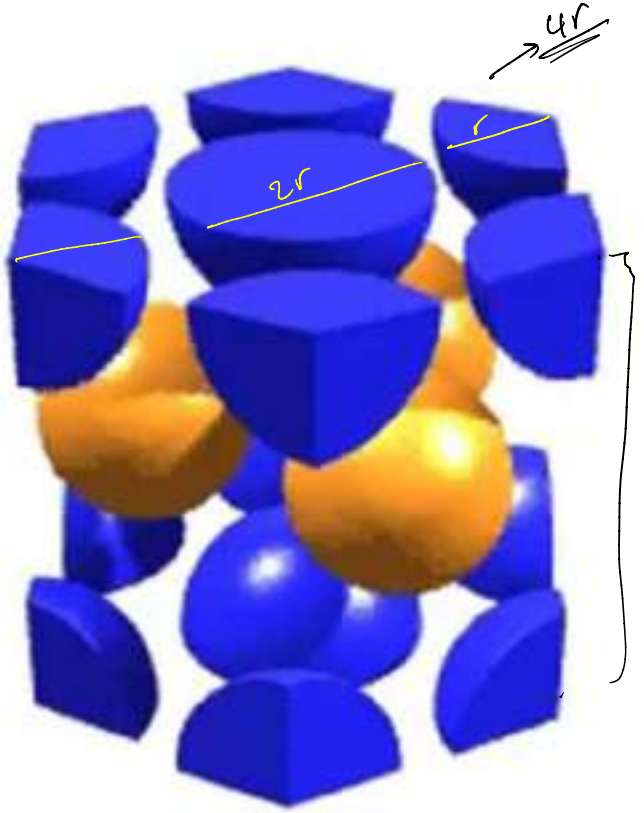


Hexagonal Close- Packed Crystal Structure

- HCP is one more common structure of metallic crystals.
- Six atoms form regular hexagon, surrounding one atom in center.
- Another plane is situated halfway up unit cell (c-axis), with 3 additional atoms situated at interstices of hexagonal (close-packed) planes.
- Example: Cd, Mg, Zn, Ti have this crystal structure.

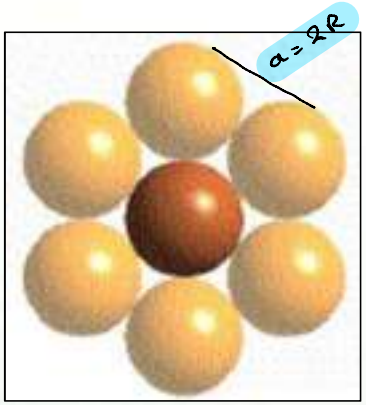


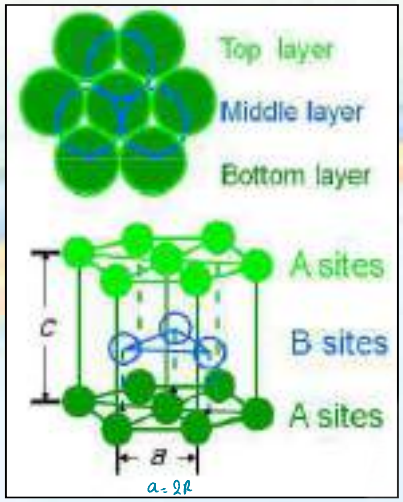
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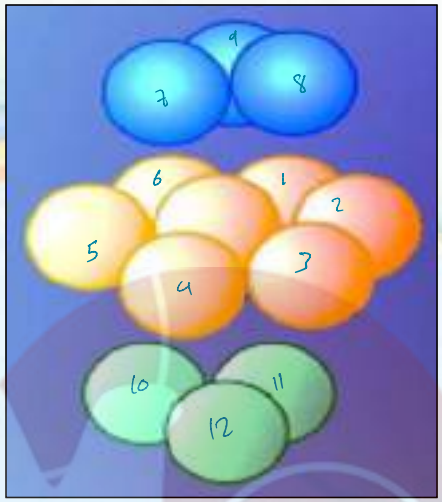


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- The hexagonal close packed structure can be made by piling layers in the A - B - A - B - A - B . . . . . sequence.
- Unit cell has two lattice parameters a and c.
- Ratio c/a = 1.633
- The coordination number, CN = 12
- Number of atoms per unit cell, n= 6.
  - ✓ 3 mid-plane atoms shared by no other cells: 3 x 1 = 3
  - ✓ 12 hexagonal corner atoms shared by 6 cells: 12 x 1/6 = 2
  - ✓ 2 top/bottom plane center atoms shared by 2 cells: 2 x 1/2 = 1







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- *In 3-D the packing efficiency is given by :*
  - ✓ *P.E. = (Volume of spheres) / (volume of cell)*

$$Volume\ of\ spheres = 6 \times \frac{4}{3} \times \frac{22}{7} \times (r)^3$$

$$Volume\ of\ spheres = 25.1428(r)^3$$

$$Volume\ of\ cell = 24\sqrt{2}(r)^3 \Rightarrow$$

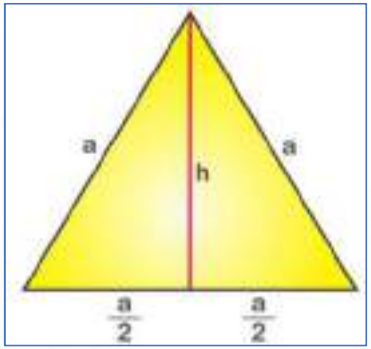
Volume = Area of triangle * c * 6 (عدد الخلايا)

$= \sqrt{3}r^2 * 3.266r \cdot 6$

$= 24\sqrt{2} = 33.9411$

$$\therefore P.E. = 0.7405$$ (نظرية)

السبب بيش هاي
نفس سيزمو أعلى
هكذا تم 12 ذرات بالوسط و 8 عند زوايا
و هو الخلية



$a^2 = h^2 + (a/2)^2$

$\Rightarrow h^2 = a^2 - a^2/4$

$\Rightarrow h^2 = (3a^2)/4$

Or, $h = \frac{1}{2}(\sqrt{3}a)$

Area of Triangle = ½ × base × height

$\Rightarrow A = \frac{1}{2} \times a \times \frac{1}{2}(\sqrt{3}a)$

$A = \frac{\sqrt{3}}{4}a^2 = \sqrt{3}r^2$

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Density Computations

⇒ Estimation based on the building block

- Since the entire crystal can be generated by the repetition of the unit cell, the density of a crystalline material,

Theoritical $$Density = \rho = \frac{Mass\ of\ Atoms\ in\ Unit\ Cell}{Total\ Volume\ of\ Unit\ Cell}$$ ⇒ Bulk ρ

(Total Volume of Unit Cell ← edge عشان الحجم بيطلع بدلالة الـ edge)

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

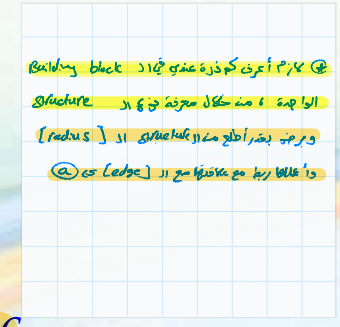
Where: n = number of atoms/unit cell

A = atomic weight

V_C = Volume of unit cell = a^3 for cubic

N_A = Avogadro's number

= 6.023×10^{23} atoms/mol



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Characteristics of Selected Elements

Actual density => mass / volume

Element	Symbol	Atomic Number	Atomic Weight (amu)	Density of Solid, 20°C (g/cm³)	Crystal Structure, 20°C	Atomic Radius (nm)	Ionic Radius (nm)	Most Common Valence	Melting Point (°C)
Aluminum	Al	13	26.98	2.71	FCC	0.143	0.053	3+	660.4
Argon	Ar	18	39.95	—	—	—	—	Inert	−189.2
Barium	Ba	56	137.33	3.5	BCC	0.217	0.136	2+	725
Beryllium	Be	4	9.012	1.85	HCP	0.114	0.035	2+	1278
Boron	B	5	10.81	2.34	Rhomb.	—	0.023	3+	2300
Bromine	Br	35	79.90	—	—	—	0.196	1−	−7.2
Cadmium	Cd	48	112.41	8.65	HCP	0.149	0.095	2+	321
Calcium	Ca	20	40.08	1.55	FCC	0.197	0.100	2+	839
Carbon	C	6	12.011	2.25	Hex.	0.071	~0.016	4+	(sublimes at 3367)
Cesium	Cs	55	132.91	1.87	BCC	0.265	0.170	1+	28.4
Chlorine	Cl	17	35.45	—	—	—	0.181	1−	−101
Chromium	Cr	24	52.00	7.19	BCC	0.125	0.063	3+	1875
Cobalt	Co	27	58.93	8.9	HCP	0.125	0.072	2+	1495
Copper	Cu	29	63.55	8.94	FCC	0.128	0.096	1+	1085
Fluorine	F	9	19.00	—	—	—	0.133	1−	−220
Gallium	Ga	31	69.72	5.90	Ortho.	0.122	0.062	3+	29.8
Germanium	Ge	32	72.64	5.32	Dia. cubic	0.122	0.053	4+	937
Gold	Au	79	196.97	19.32	FCC	0.144	0.137	1+	1064
Helium	He	2	4.003	—	—	—	—	Inert	−272 (at 26 atm)
Hydrogen	H	1	1.008	—	—	—	0.154	1+	−259
Iodine	I	53	126.91	4.93	Ortho.	0.136	0.220	1−	114

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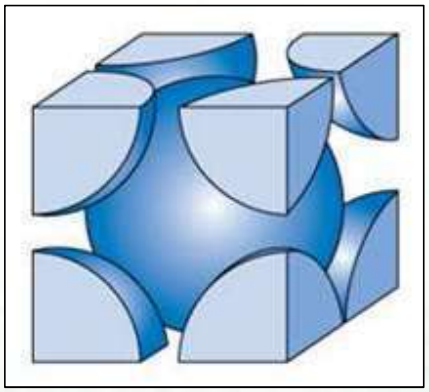
Theoretical Density, ρ

- Ex: Cr (BCC)

$\mathcal{A} = 52.00\ g/mol$

$\mathcal{R} = 0.125nm$

$n = 2$



$$a = \frac{4}{\sqrt{3}}R$$

$$a = \frac{4}{\sqrt{3}}(0.125) = 0.2887\ nm$$

$$\rho = \frac{2 \times 52.0}{(0.2887 \times 10^{-9})^3 \times 6.023 \times 10^{23}} = 7175961.9\ \frac{g}{nm^3}$$

$$\rho = 7175961.9\ \frac{g}{m^3}\frac{m^3}{(100\ cm)^3} = 7.176\ \frac{g}{cm^3}$$ *Theoretical*

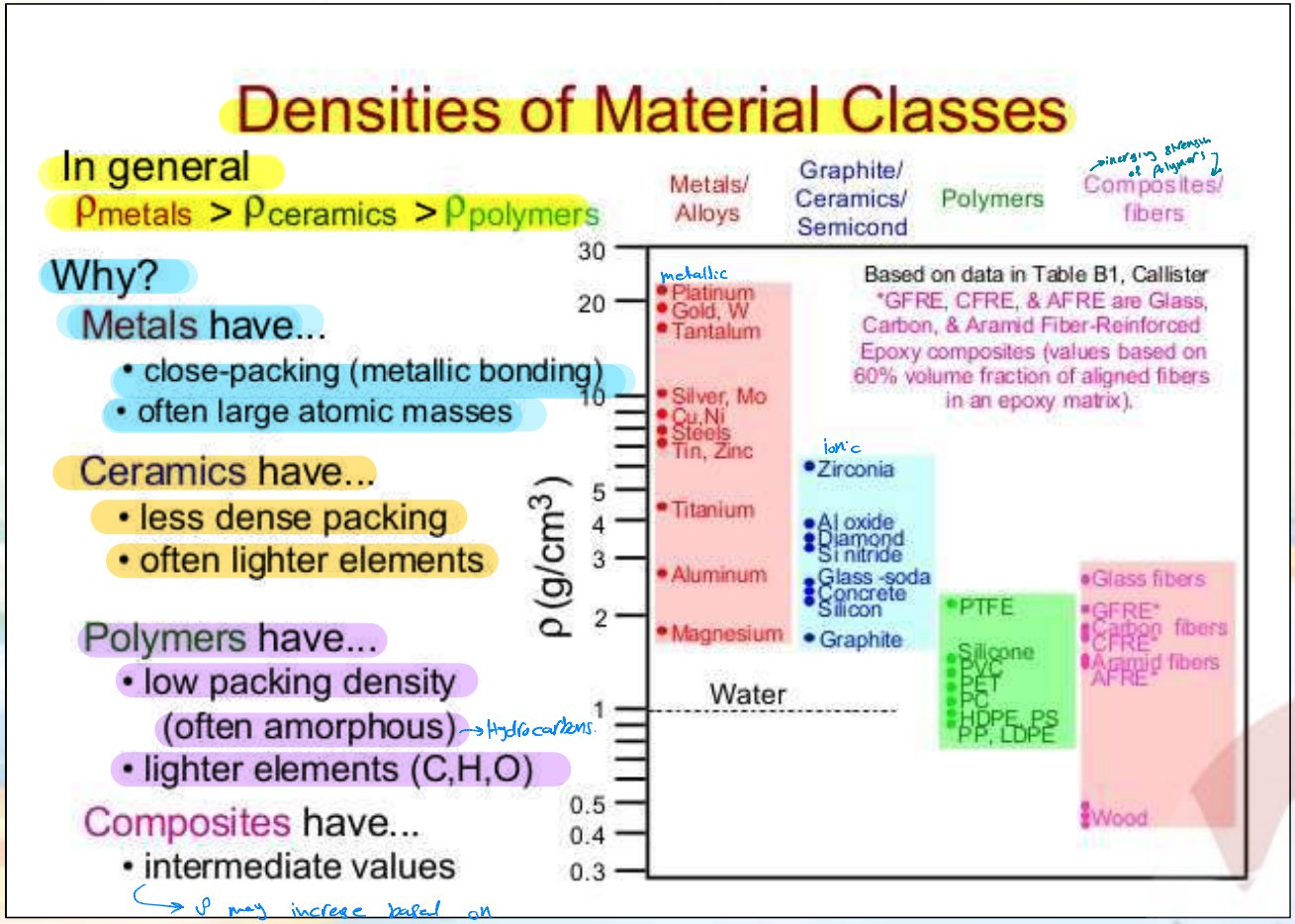
The actual density is 7.19

* ليش في اختلاف بين القيمة النظرية والفعلية ؟

لأننا احنا أخذنا افتراض إنه الذرات عبارة عن spheres 100% [pure element] في الكتيبة - هو ٨. والعامل الأهم للاختلاف إنه عندي في المختبر حتى لو pure بس فيها impurities .

ممكن تكون هاي الذرات بدل ما أخت بدل ما أثقل .

Densities of Materials Classes



Chapter 3

The Structure of Crystalline Solids Part B

The University of Jordan
Chemical Engineering Department
First Semester 2021
Prof. Yousef Mubarak

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Outline

- Crystals as Building Blocks
- Isotropic OR Anisotropic
- Polymorphism and Allotropy
- Crystallographic Points, Directions, and Planes
  1. Symmetry Equivalent Directions
  2. POINT Coordinates
  3. Direction Coordinates
  4. How Do We Designate Lattice Planes?
- Linear Density
- Planar Density
- Designating Lattice Planes

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Crystals as Building Blocks

- Some engineering applications require single crystals:

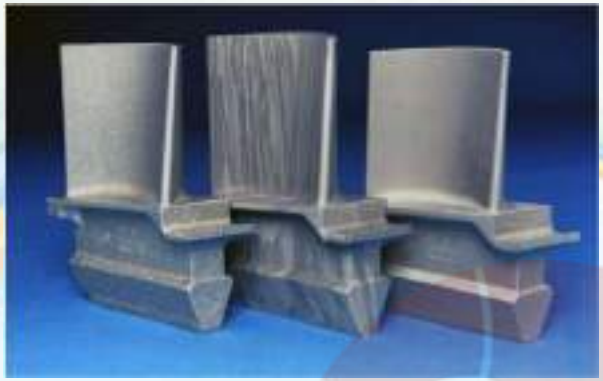
Diamond single crystals for abrasives





- Properties of crystalline materials often related to crystal structure.

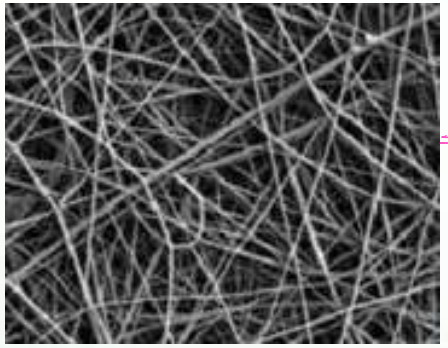
Ex: Quartz fractures more easily along some crystal planes than others.

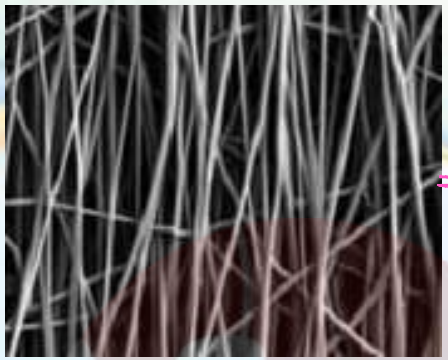


Turbine blades

Polycrystalline Materials

- Most engineering materials are polycrystalline.
- In polycrystalline materials, grain orientations are random, so bulk material properties are isotropic. => bulk similar properties in all directions. (based on orientation) => selection also based on the application
  Anisotropic => having different properties in each direction
- Some polycrystalline materials have grains with preferred orientations (texture), so properties are dominated by those relevant to the texture orientation.
- If grains are randomly oriented, overall component properties are not directional.



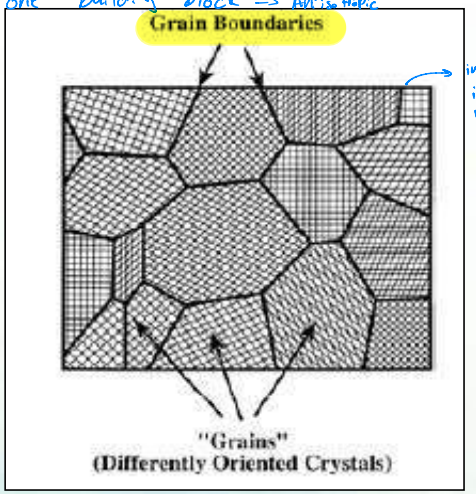


Yousef Mubarak

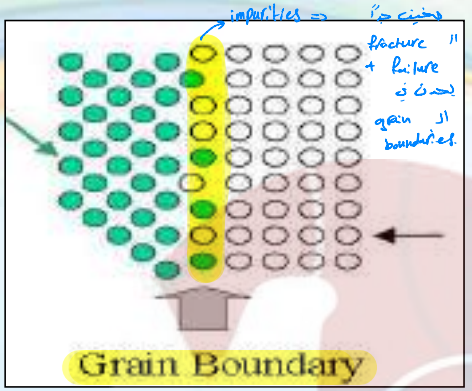
Single Crystals and Polycrystalline Materials

- *Single crystal:* atoms are in a repeating or periodic array over the entire extent of the material.
- *Polycrystalline material:* comprised of many small crystals or grains. The grains have different crystallographic orientation.
- There exist atomic mismatch within the regions where grains meet. These regions are called grain boundaries.

one building block => Anisotropic



in each crystal in this picture has a different orientation than the others
so its a anisotropic but for the bulk its isotropic
so these two definitions are mixed in polycrystalline structure => based on the scale we choose it will vary.



size of crystals depends on the cooling rate
as the cooling rate ↑ the size of crystals will be ↓
Also, it depends on the other nucleating agents



عند نمو الكريستالات
أحد نقطة التقاء بينهم لتنمو
impegement Point ال
هنا لا يتوقف نمو هذه الكريستالات من هذه النقطة.
grain boundaries لا يعبر عن فاصل بينهم التي هو ال

Length of grain boundaries ↑ when

1) number of crystals ↑ and their size is ↓

* هي التي يظهر بين التقاء الكريستالات خط مستقيم
انا جعل هذا خلع مستقيم و ممكن أشكال أخرى
مهمة جداً لماذا نحن نحدد ال properties

خلع خط مستقيم لأنه ال growth rate ثابت
عند

1) growth rate
2) type of crystal.

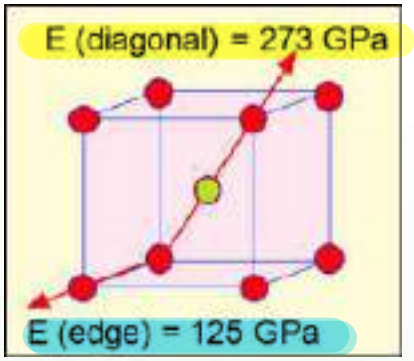
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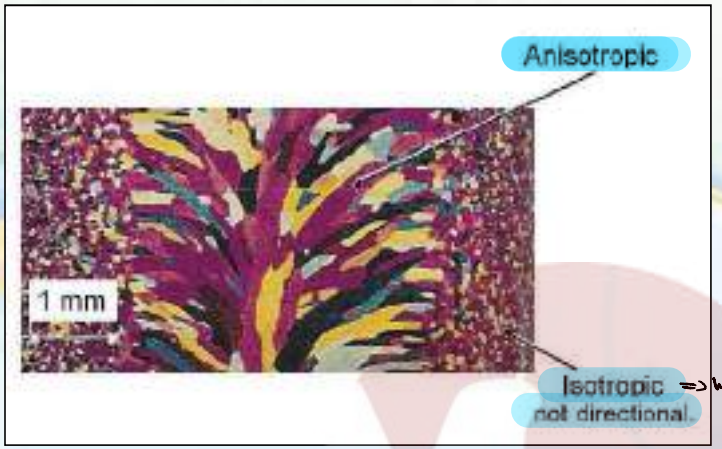
Single Crystals

- Properties vary with direction: anisotropic. => why ? because of different of contacts between the atoms in one crystals (num , kinds _ etc)
- Example: the modulus of elasticity E in BCC iron.
  - resistance of material of deformation in the elastic region



Polycrystals

- Properties may/may not vary with direction.
- If grains are randomly oriented: isotropic. ($E_{poly\ iron}$ = 210 GPa)
- If grains are textured, anisotropic.



Isotropic OR Anisotropic

- **Anisotropic** exhibiting properties with different values when measured along axes in different directions.

- **Isotropic** exhibiting properties with the same values when measured along axes in all directions.

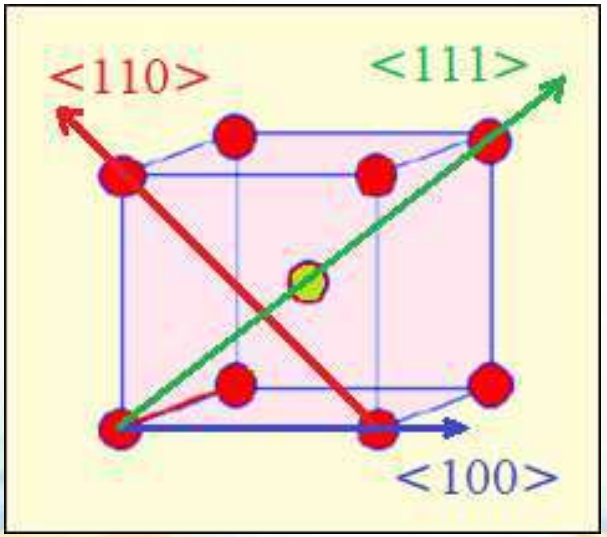
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Anisotropy

- Different directions in a crystal have different packing.
- For instance, atoms along the edge of FCC unit cell are more separated than along the face diagonal.
- This causes anisotropy in the properties of crystals, for instance, the deformation depends on the direction in which a stress is applied.
- In some polycrystalline materials, grain orientations are random, so bulk material properties are isotropic

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- *Some polycrystalline materials have grains with preferred orientations (texture), so properties are dominated by those relevant to the texture orientation and the material exhibits anisotropic properties.*
- *Properties of crystals may be different along different directions, because atomic periodicities are different.*
- *E.g. in single crystal cubic system:*



- *< 100 > Cube edges*
- *< 110 > Face diagonals*
- *< 111 > Body diagonals*

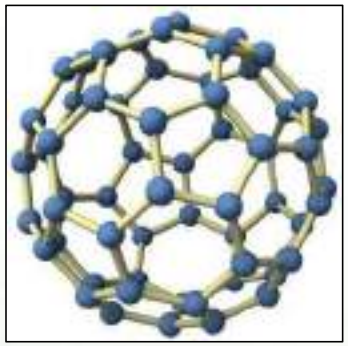
لاحظ إنه اعتادة تزيد إذا المسافة أبعد
يعني صورة بال أكيد سفوسفها عالية عشان المسافة
صبّة كبيرة .
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Polymorphism and Allotropy

- Some materials may exist in more than one crystal structure, this is called polymorphism. on different State
- If the material is an elemental solid, it is called allotropy. → but in the same state.
- Allotropy means the existence of a substance in two or more different forms in the same phase.
- An example of allotropy is carbon, which can exist as diamond, graphite, and amorphous carbon.

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- *Pure, solid carbon occurs in three crystalline forms-diamond, graphite; and large, hollow fullerenes.*
- *Two kinds of fullerenes are shown here:*
  1. *buckminsterfullerene (Buckyball)*
  2. *carbon nanotube.*



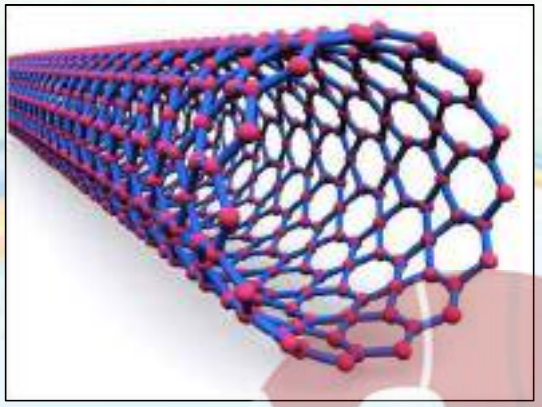
Buckyball



Graphite



Diamond



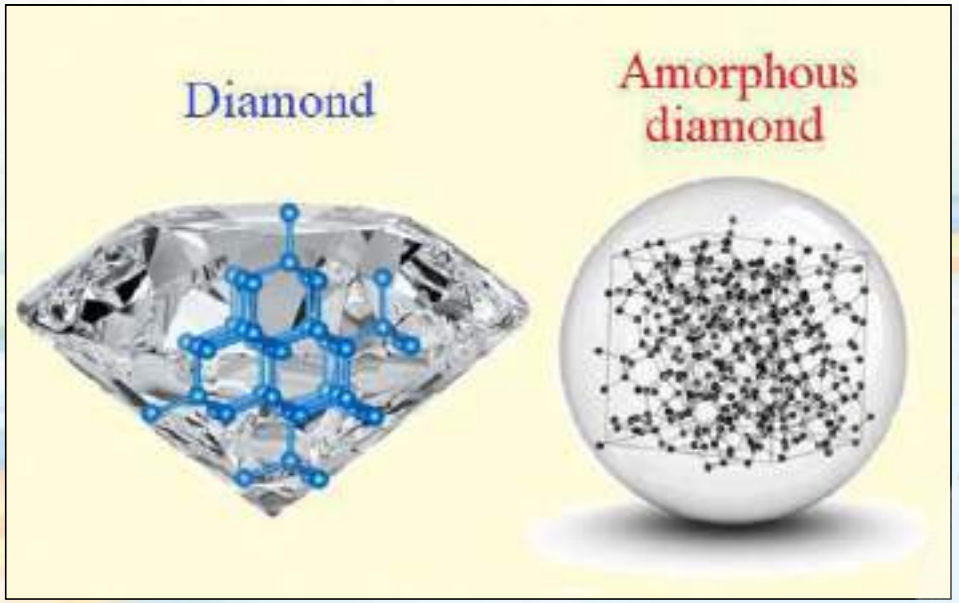
Carbon nanotube

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Non-Crystalline (Amorphous) Solids

↳ There is a arrangement but there is lack ↳ ما يتوصل لمرحلة كريستالية

- *In amorphous solids, there is no long-range order.*
- *But amorphous does not mean random, in many cases there is some form of short-range order.*



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Crystallographic Points, Directions, and Planes

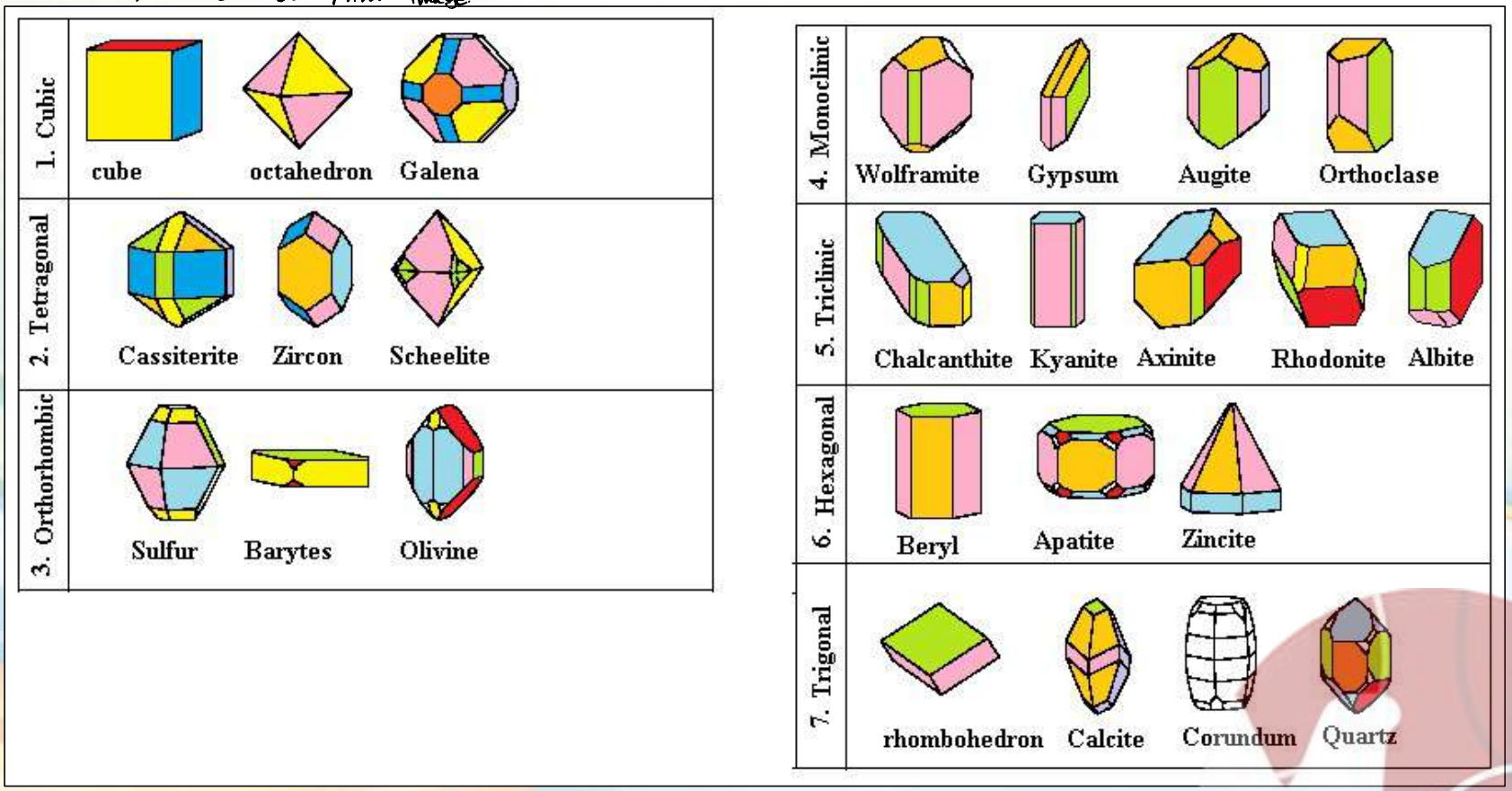
- How to define points, directions, planes, as well as linear, planar, and volume densities.
  - ✓ Points (atomic positions)
  - ✓ Vectors (defines a particular direction – plane normal)
  - ✓ Miller Indices (defines a particular plane) relation to diffraction
  - ✓ 3-indices for cubic and 4-indices notation for HCP

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→ these Building blocks have Symmetry

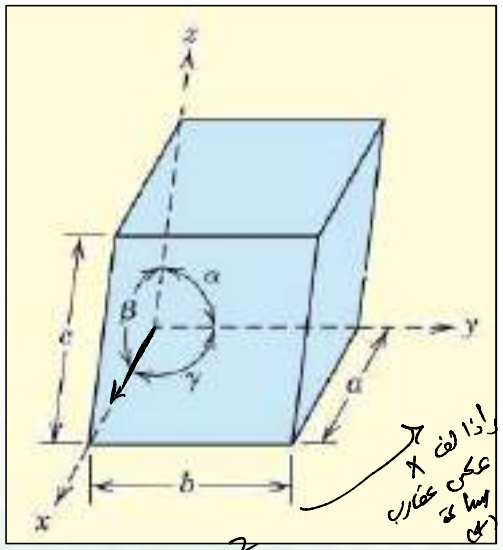
Symmetry Equivalent Directions

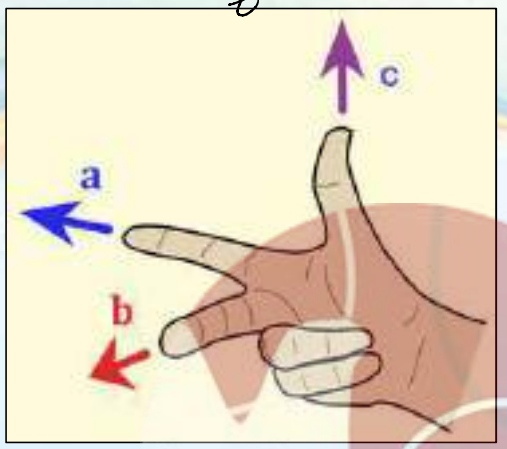
↳ we can do mirror image



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- All periodic unit cells may be described via these vectors and angles, if and only if a, b, and c define axes of a 3D coordinate system.
- Coordinate system is Right-Handed.
- We can define points, directions and planes with a "triplet" of numbers in units of a, b, and c unit cell vectors.
- For HCP we need a "quad" of numbers.



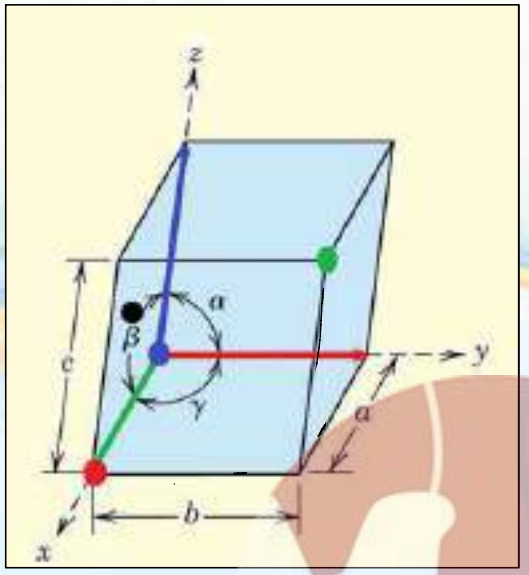


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POINT Coordinates ⇒ location of atom in building block.

- To define a point within a unit cell….
- Express the coordinates uvw as fractions of unit cell vectors a, b, and c (so that the axes x, y, and z do not have to be orthogonal).

	Pt. coordinate		
Point	x(a)	y(b)	z(c)
Blue	0	0	0
Red	1	0	0
Green	1	1	1
Black	1/2	0	1/2



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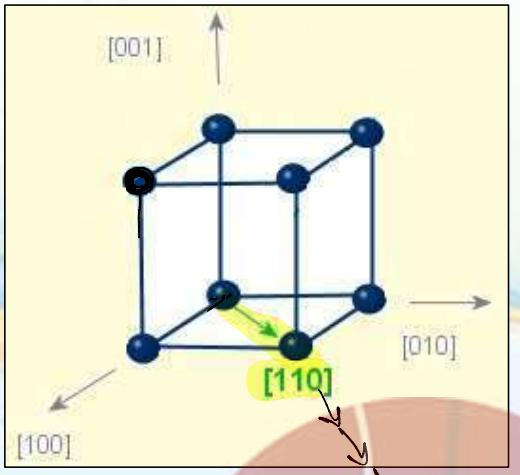
Direction Coordinates

=> we need to specify an arrow with a head and tail (reference point)

Procedure:

1. Any line (or vector direction) is specified by 2 points.
   - ✓ The first point is, typically, at the origin (000).
2. Determine length of vector projection in each of 3 axes in units (or fractions) of a, b, and c.

X(a)	Y(b)	Z(c)
1	1	0



3. Multiply or divide by a common factor to reduce the length to the smallest integer values, u v w.
4. Enclose in square brackets: [u v w]: [110] direction.
5. Designate negative numbers by a bar $[\bar{1}\,\bar{1}\,0]$
   - ✓ Pronounced "bar 1", "bar 1", "zero" direction.
6. "Family" of [110] directions is designated as <110>.

→ Same direction but in different location of points.

Direction Coordinates

What is the crystallographic direction of the red arrow?

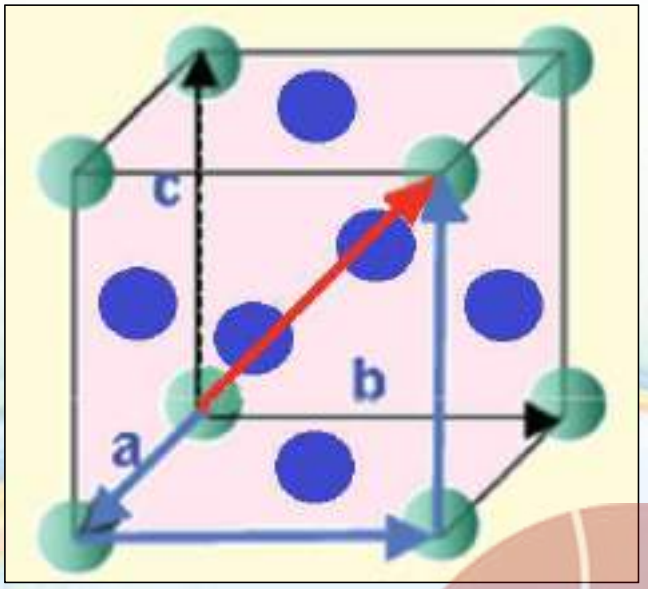
Solution:

Along x: 1 a

Along y: 1 b

Along c: 1 C

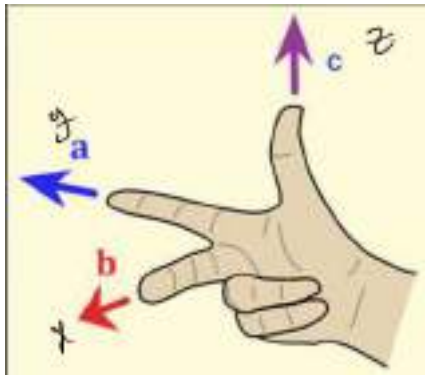
Direction = [1 1 1]



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Basic rules to determine points, direction :

1) axes :-



لقدر أختار أي محور ليكون الـ X-axis بس عشان أقدر أختار الـ y-axis لازم أتأكد اتجاه محور الـ X يتحرك لليمين عكس عقارب الساعة باتجاه الـ y ، أما بالنسبة لـ Z-axis فهو المحور العمودي عليهم .

2) points :

1) بالبداية لا لازم أحدد نقطة مرجعية ويكون احداثياتها 000 عشان أبني أساسها ومنه أحدد باقي النقاط .

2) النقطة بحددها بناءً على بُعدي عن الـ reference point و الوحدة تبعت المسافة ويكون الـ unit بالأساس بقيس على مستوى الـ Building block الواحدة فلو كانت مثلاً عندي نقطة تبعد 2 units عن الـ X-axis فهون أنا بحكي إنه Building blok في ثانية بجانب الأول وهكذا .

3) التعبير عن النقطة يكون باستخدام الأرقام دون حواجز أو أقواس ← 100 مثل هيك .

3) directions :-

1) عند تحديد الاتجاه أنا بروح راسم خط ذهني في الـ ref. point وراسم عن النقطة إلي بدي أطلع الاتجاه عندها

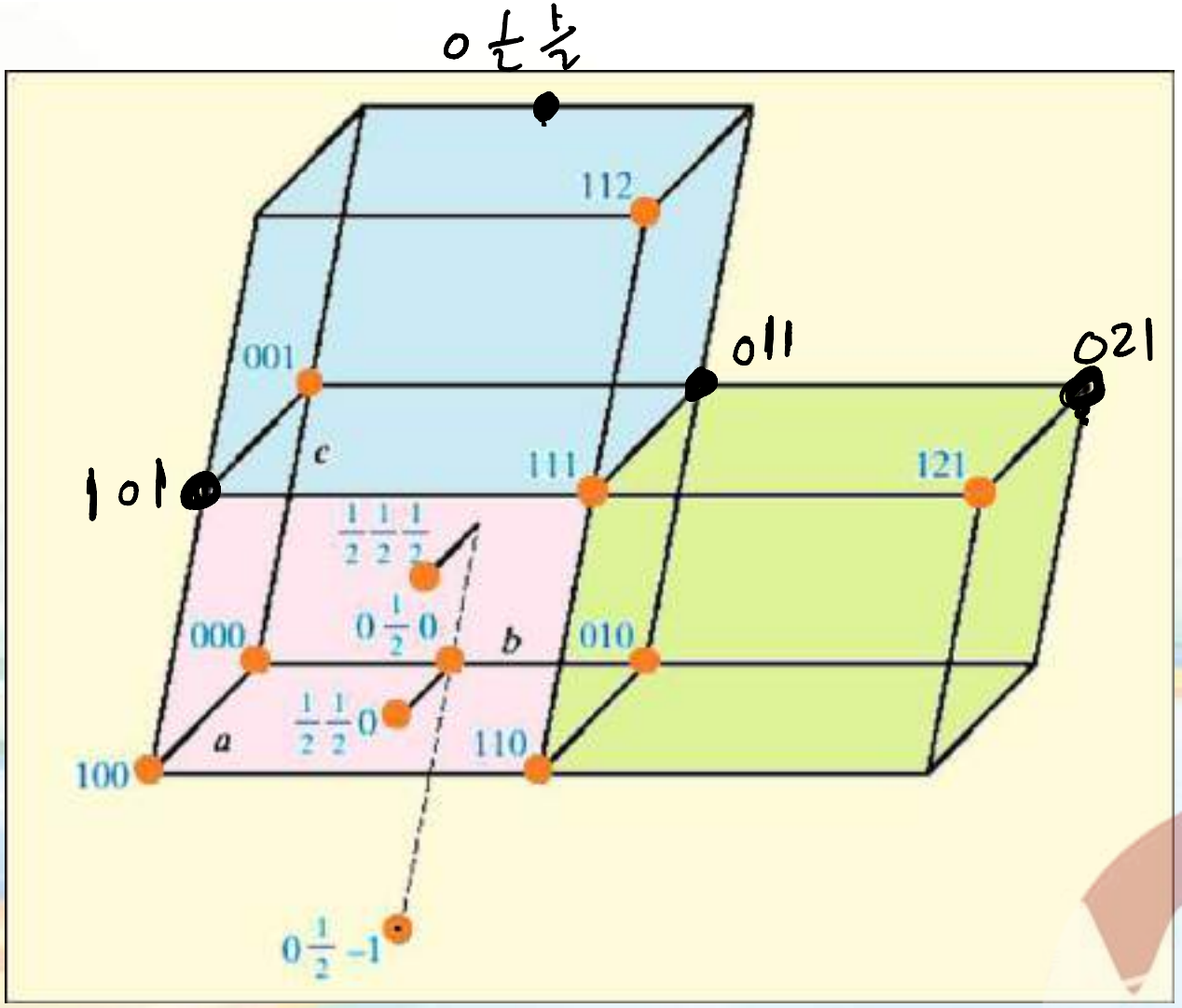
2) بدي أحدد طولهم يعني صبأ الـ points

3) لازم أقسم أو أضرب عشان أحصل على أحد (integer) ← يعني هستخدم عند تحديد الاتجاه في الجواب النهائي يكون في frac في زي الـ points !!!

4) لازم نبسط الجواب النهائي بين قوسين [100] وبعد التبسيط .

5) عند تغير في الاحداثيات السالبة نضع Bar فوق الرقم

6) ممكن أكثر من نقطة تقع على نفس الاتجاه والتغير عنهم يكون < 110 > ← زي هيك



adar
ask :: believe & recieve

Point and Direction Coordinates

a) What is the lattice point given by point P?

Solution:

$\bar{1}$ 1 2

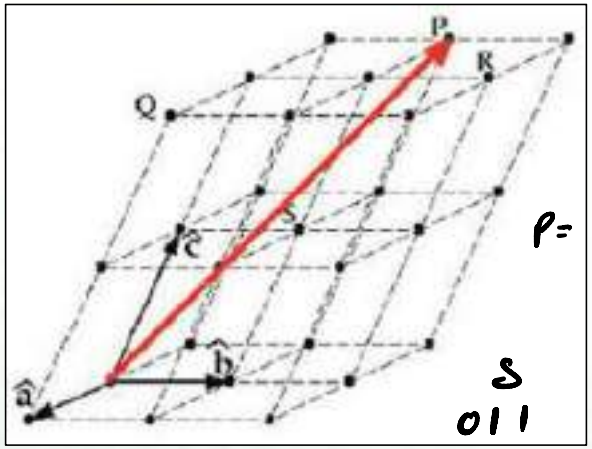
b) What is the crystallographic direction for the origin to P?

Solution:

$[\bar{1}\ 1\ 2]$

264

= 132



P= $\bar{1}$ 1 2

S 0 1 1

R => 0 2 2

Q = 1 0 2

c) What lattice direction does the lattice point 264 correspond?

Solution:

The lattice direction [1 3 2] from the origin

Madar ask :: believe & recieve

Symmetry Equivalent Directions

Note: for some crystal structures, different directions can be equivalent.

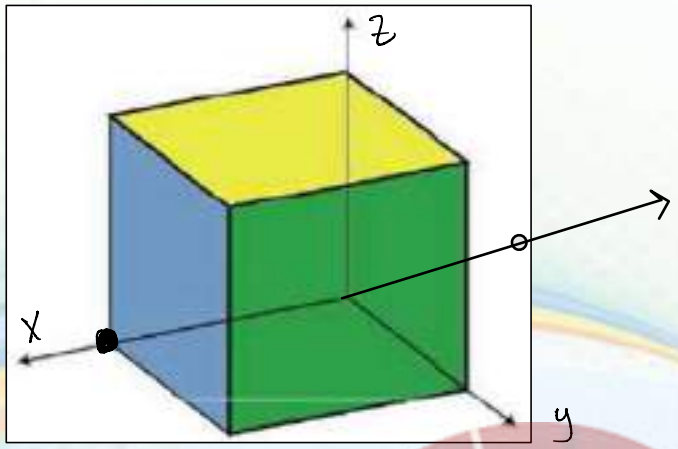
e.g. For cubic crystals, the directions are all equivalent by symmetry:

$[1\ 0\ 0], [\bar{1}\ 0\ 0], [0\ 1\ 0],$
$[0\ \bar{1}\ 0], [0\ 0\ 1], [0\ 0\ \bar{1}]$

معكن يكونو كل معدل مو نفس اتجاه و لاحظ [100]

كيف في من حالين تغير اتجاه /

They are results of rotation of the building block



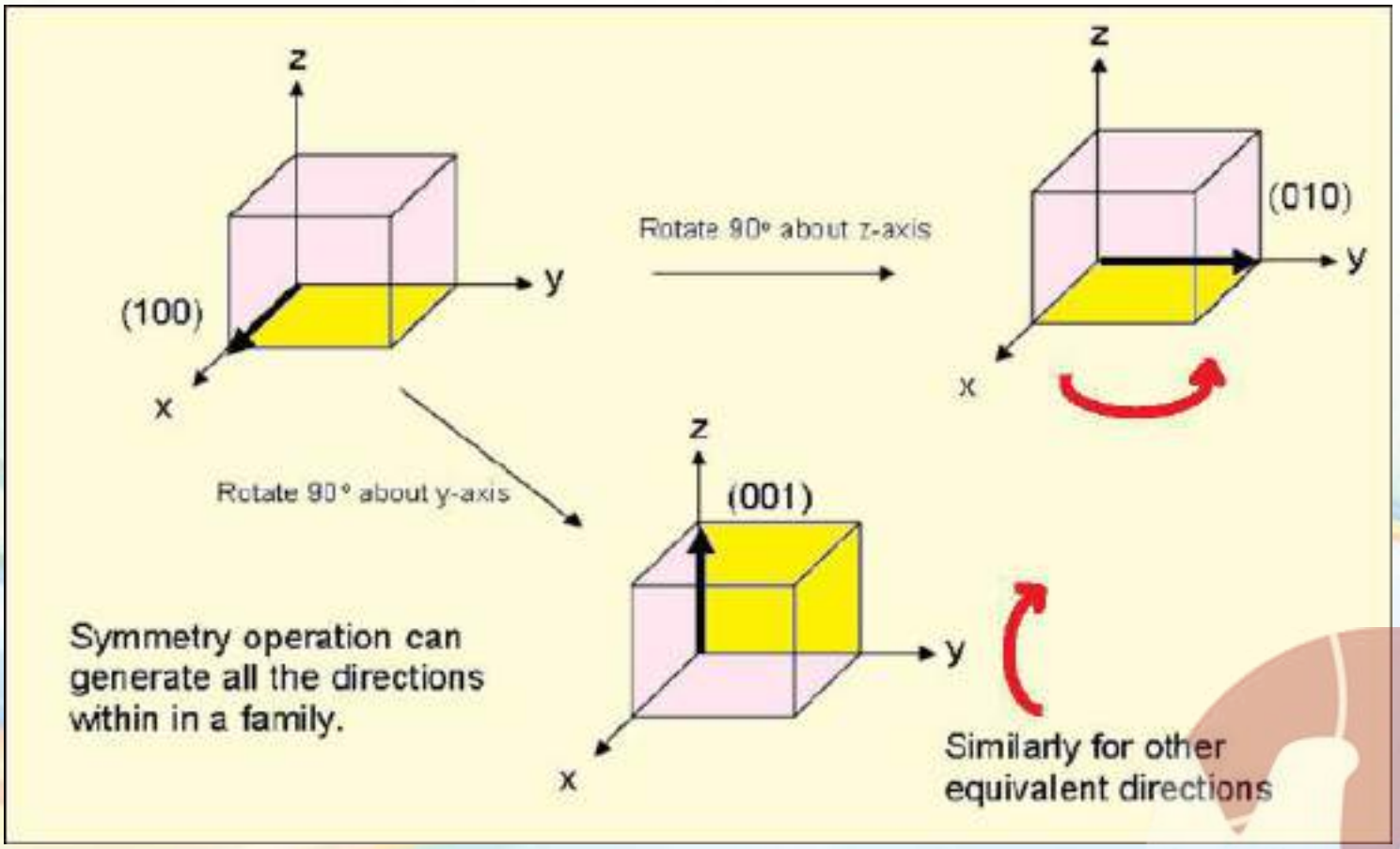
Families of crystallographic directions

e.g. $<1\ 0\ 0>$ → it includes the rest families of <100> taking the all alternatives of rotation.

Angled brackets denote a family of crystallographic directions

adar ask :: believe & recieve

Symmetry Equivalent Directions



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How Do We Designate Lattice Planes?

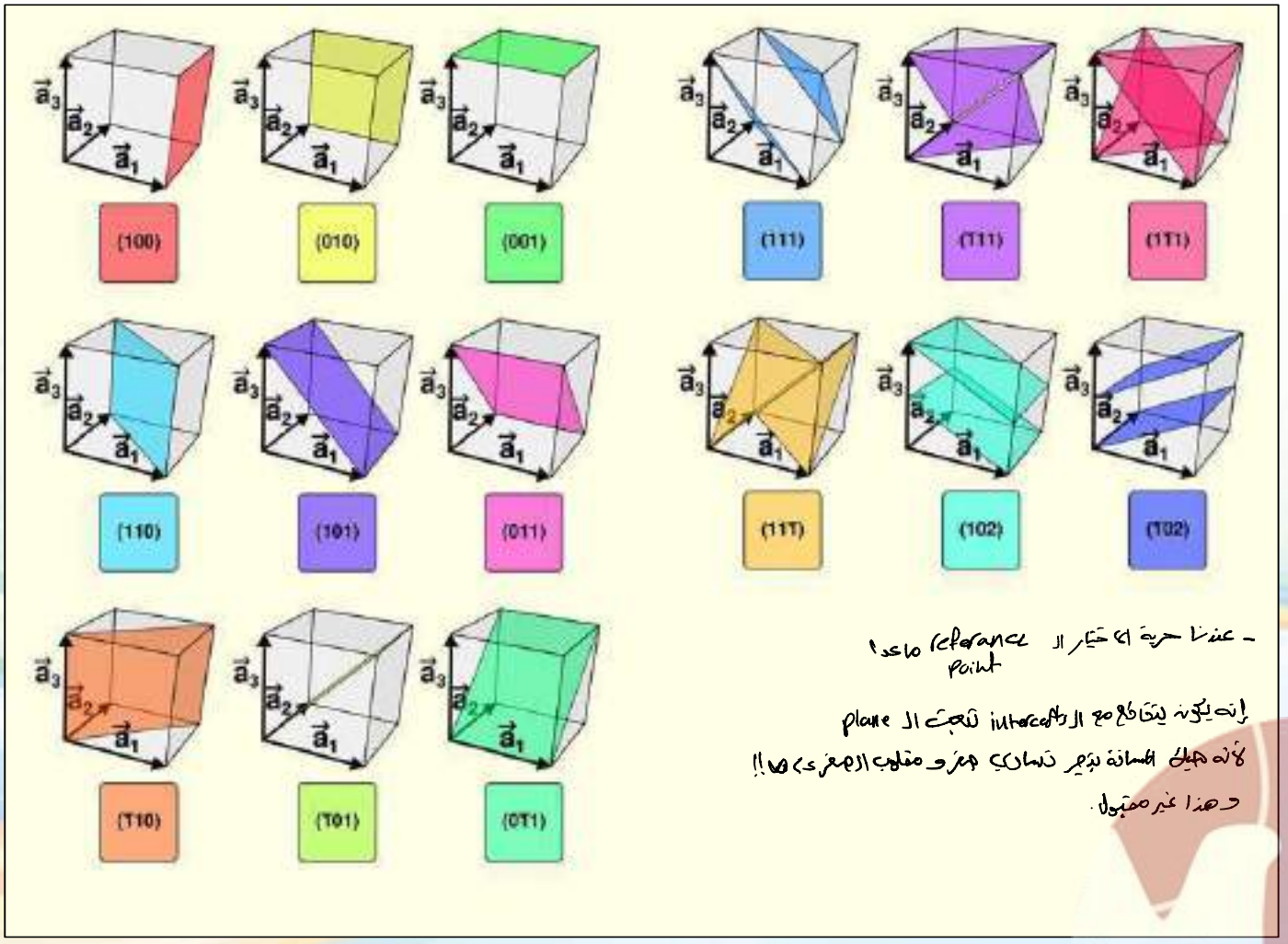
Crystallographic Planes

- Miller Indices: Reciprocals of the (three axial intercepts for a plane, cleared of fractions and common multiples.
- All parallel planes have same Miller indices.

Algorithm

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

adar ask :: believe & recieve

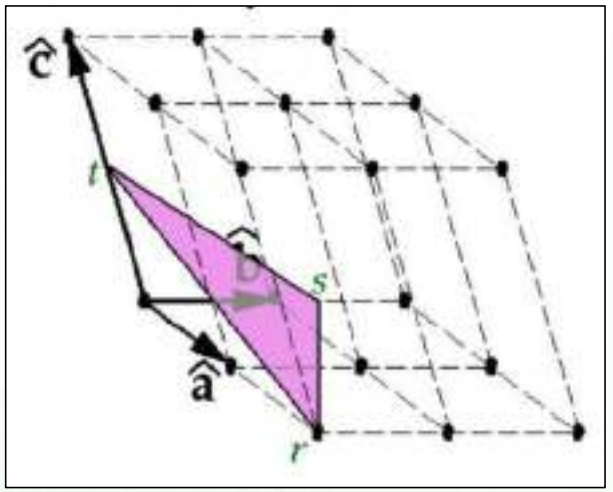


- عندنا حرية اختيار الـ reference point ماعدا إنه يكون يتقاطع مع الـ plane intercepts لأنه هيبقى المسافة بيبقى تساوي صفر وهذا غير مقبول.

Radar ask :: believe & recieve

Planes intersects axes at:

- a axis at r = 2
- b axis at s = 4/3
- c axis at r = ½



How do we symbolically designate planes in a lattice?

1. Take the reciprocal of r, s, and t.
   Here: 1/r = ½, 1/s = ¾, and 1/t = 2
2. Find the least common multiple that converts all reciprocals to integers.
   With LCM = 4, h = 4/r = 2, k = 4/s = 3, and l = 4/t = 8
3. Enclose the new triple (h, k, l) in parentheses: (2 3 8)
4. This notation is called the Miller Index.

Note 1: if a plane does not intercept an axes (i.e., it is at ∞), then you get 0.

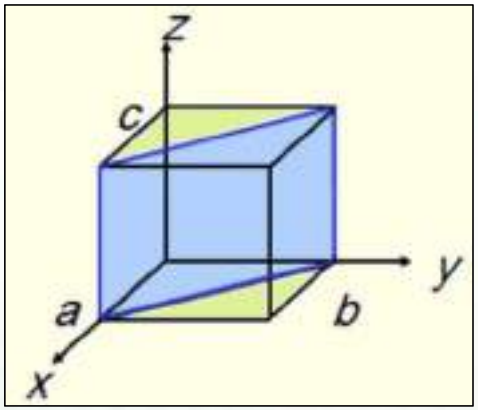
Note 2: All parallel planes at similar staggered distances have the same Miller Index.

Crystallographic Planes

Example 1

	a	b	c
Intercepts	1	1	∞
Reciprocals	1/1 1	1/1 1	1/∞ 0
Reduction	1	1	0

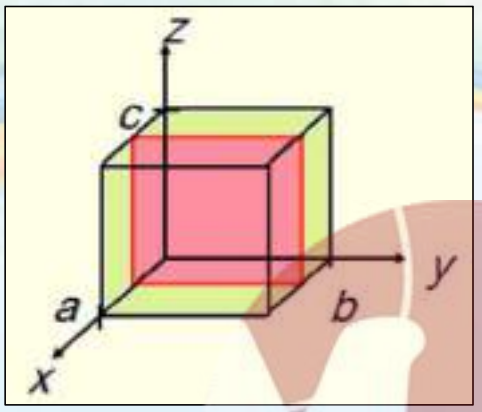
Miller Indices: (1 1 0)



Example 2

	a	b	c
Intercepts	1/2	∞	∞
Reciprocals	1/(1/2) 2	1/∞ 0	1/∞ 0
Reduction	2	0	0

Miller Indices: (2 0 0)

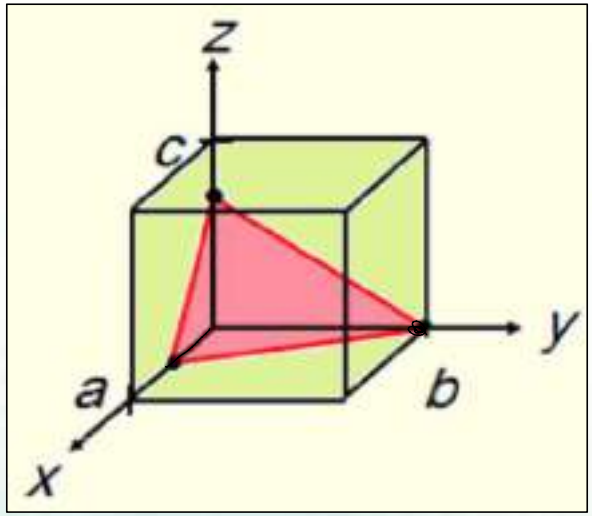


Crystallographic Planes

Example 3

	a	b	c
Intercepts	1/2	1	3/4
Reciprocals	1/(1/2) 2	1/1 1	1/(3/4) 4/3
Reduction	6	3	4

Miller Indices: (6 3 4)



Family of Planes {h k l}

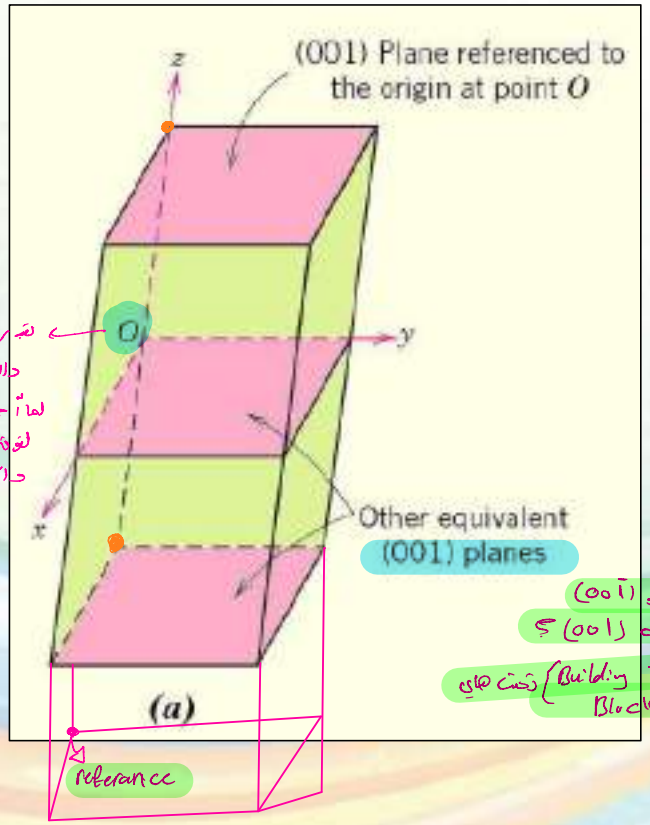
Ex: {1 0 0} = (1 0 0), (0 1 0), (0 0 1), $(\bar{1}\ 0\ 0)$, $(0\ \bar{1}\ 0)$, $(0\ 0\ \bar{1})$

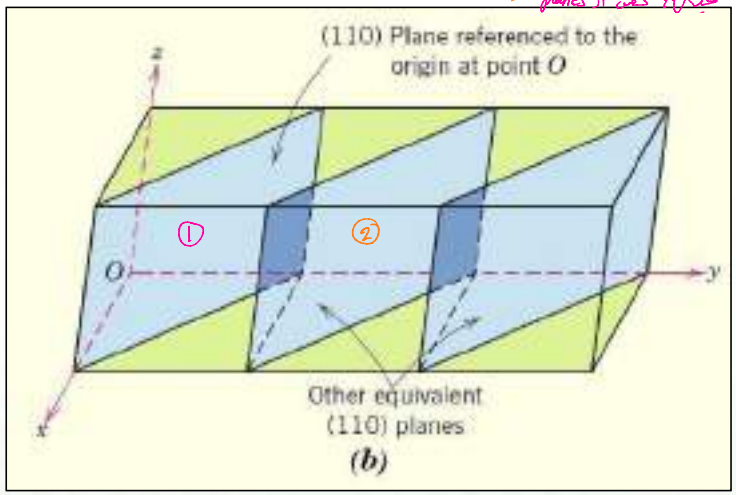
adar
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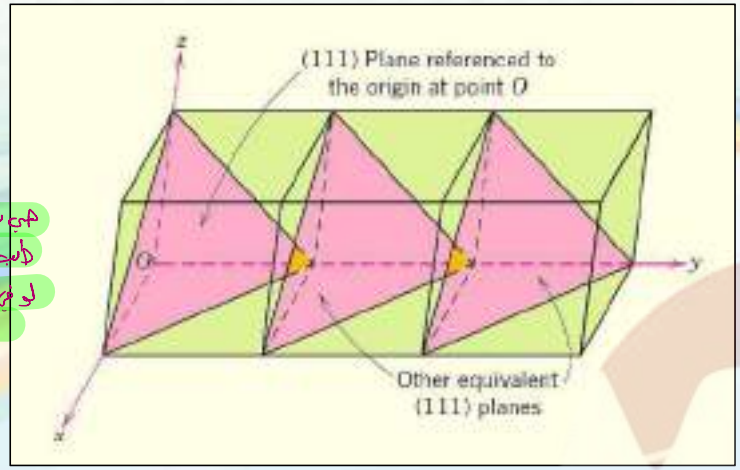
	x	y	z
d	1	1	∞
R	1	1	1/∞
	(1	1	0)

x	y	z	
2	2	∞	
1/2	1/2	1/∞	
1/2	1/2	0	
(1	1	0)	

Same plane!!



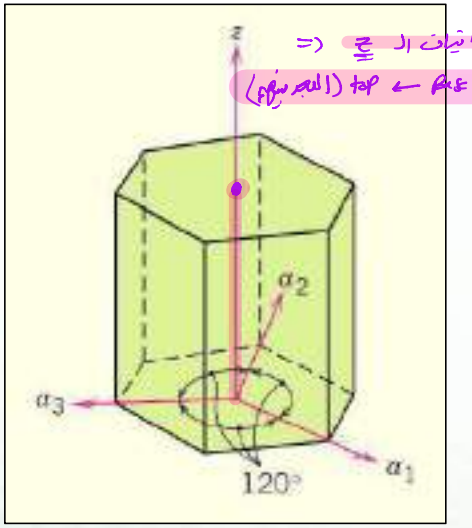


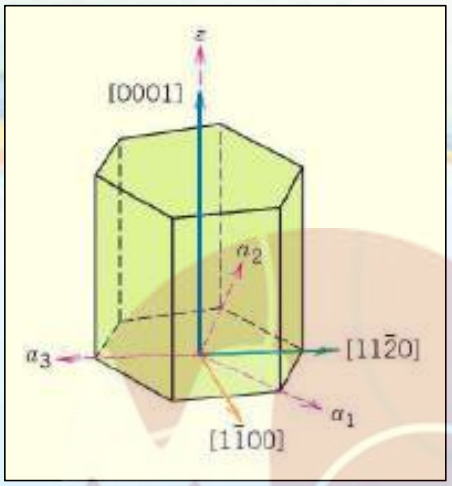


HCP Crystallographic Directions

Algorithm

1. Vector repositioned (if necessary) to pass through origin.
2. Read off projections in terms of unit cell dimensions a_1, a_2, a_3, or c
3. Adjust to smallest integer values
4. Enclose in square brackets, no commas [u v t w].

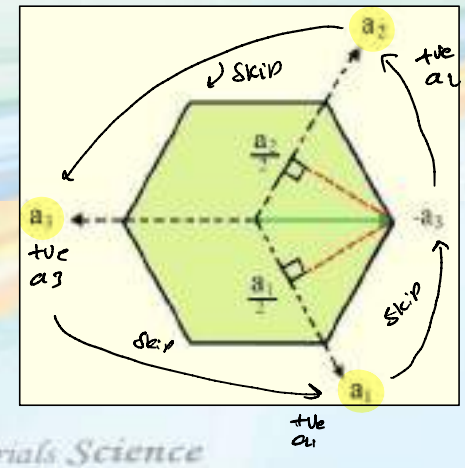




Ex:

½, ½, -1, 0 ⟹ [1 1 $\bar{2}$ 0]

Dashed red lines indicate projections onto a_1 and a_2 axes



The three numbers are parameters $(\acute{u}, \acute{v}, \acute{w})$

$\acute{w}$ = vertical distance between head and tail.

$\acute{u}, \acute{v}$ => projection of the head on the tail or it's extension on $(\bar{a}_3, a_1)$ => for $\acute{u}$ or on $(\bar{a}_2, a_2)$ => for $\acute{v}$

HCP Crystallographic Directions

Hexagonal Crystals

4 parameter Miller-Bravais lattice coordinates are related to the direction indices (i.e., ú v́ ẃ) as follows.

$[\acute{u}\ \acute{v}\ \acute{w}] \rightarrow [u\ v\ t\ w]$

$$u = \frac{1}{3}(2\acute{u} - \acute{v})$$

$$v = \frac{1}{3}(2\acute{v} - \acute{u})$$

$$t = -(u + v)$$

$$w = \acute{w}$$

!! لاحظ الترتيب

$[\acute{u}\ \acute{v}\ \acute{w}] = [1\ 1\ 0]$

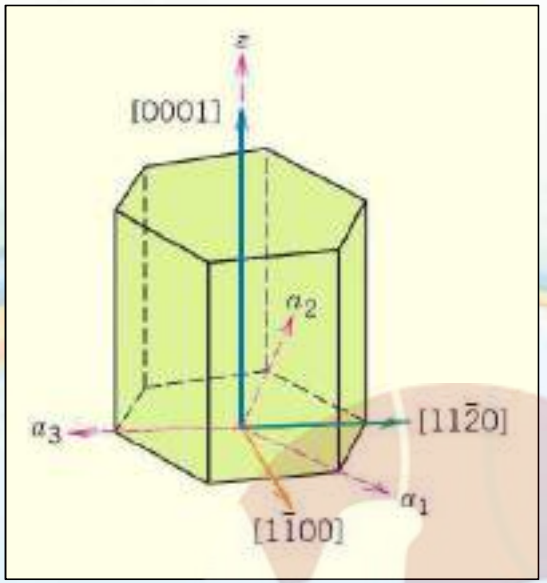
$$u = \frac{1}{3}(2 \times 1 - 1) = \frac{1}{3}$$

$$v = \frac{1}{3}(2 \times 1 - 1) = \frac{1}{3}$$

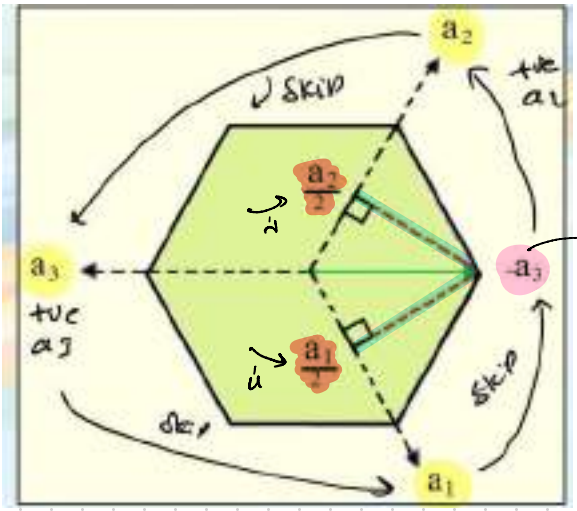
$$t = -\left(\frac{1}{3} + \frac{1}{3}\right) = -\frac{2}{3}$$

$$w = 0$$

$$\left[\frac{1}{3}\ \frac{1}{3}\ \frac{-2}{3}\ 0\right] = [1\ 1\ \bar{2}\ 0]$$



Radar ask & believe & recieve



نسقط w على a2 و a1 ونكون الاتجاهين موازيين للبعد

اسقاط رأس a3 على القاعدة

* عشان أحدد ال Direction بشكل صحيح لازم أحدد ٣ أرقام بحيث يتحقق فيها داخل معادلات ٥

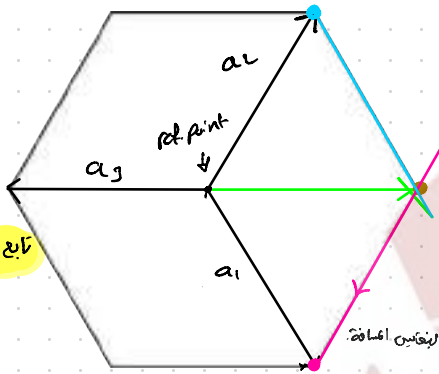
The three numbers are parameters (ú, ṕ, ẃ)

ẃ = vertical distance between head and tail.

ú, ṕ => projection of the vector on the Base of Hexagon

(يتم حلها بطريقة المعادلات لتحديد النقاط أو الاتجاه)

مثال في الرسمة إني خوفته شو فيه ٥



=> ẃ = 0

لأنه أعلى الرسم على الأرضية ما أسقطنا على المحاور.

=> ú = 1

موازي لـ a2 ما يقطع على a1 أو امتداده (a1) لبعدين اضافة

ṕ = 1

نفس الشي ولكن لـ a2

لـ الخط الموازي لـ a1 ويقطع لـ a2 أو امتداده

$t = -(\frac{1}{3} + \frac{2}{3})$

تابع ٥

$[u\ v\ w] = [1\ 1\ 1]$

to find $[u\ v\ t\ w]$

$u = \frac{1}{3}(2t\acute{u} - \acute{v})$

$u = \frac{1}{3}(2 - 1)$

$\boxed{u = \frac{1}{3}}$

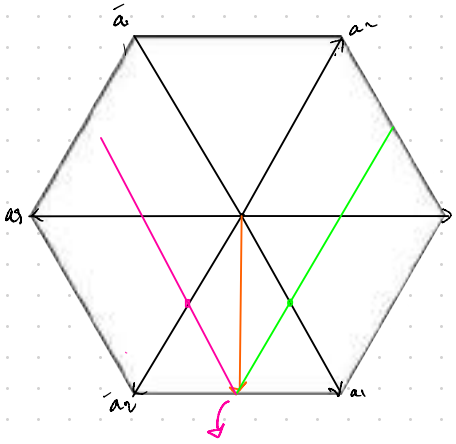
$v = \frac{1}{3}(2\acute{v} - \acute{u})$

$v = \frac{1}{3}$

$t = -(\frac{1}{3} + \frac{1}{3}) = \frac{-2}{3}$

$w = \acute{w} = 0$

$[\frac{1}{3}\ \frac{1}{3}\ \frac{-2}{3}\ 0] \Rightarrow [1\ 1\ \bar{2}\ 0]$



لتحديد ⇐ الخط الموازي لـ a_2 و امتداده بحيث يقطع $\dot{u}$ أو امتداده هيلغ بكون ملتصق
و العكس لـ لأن ⇐

$\Rightarrow \dot{w} = 0$

$\dot{u} = 0.5$

$\dot{v} = -0.5$

$[\dot{u}\ \dot{v}\ \dot{w}] = [0.5\ -0.5\ 0]$

$u = \frac{1}{3}[2\dot{u} + \dot{v}]$

$u = \frac{1}{3}[1 - 0.5]$

$u = \frac{1}{6}$

$v = \frac{1}{3}[2\dot{v} + \dot{u}]$

$v = \frac{1}{3}[-1 + 0.5]$

$v = \frac{-1}{6}$

$t = -(-\frac{1}{6} + \frac{1}{6})$

$t = 0 \qquad w = \dot{w} = 0$

$[\frac{1}{6}\ \frac{-1}{6}\ 0\ 0]$

$\pm[1\ \bar{1}\ 0\ 0]$

adar
ask & believe & recieve

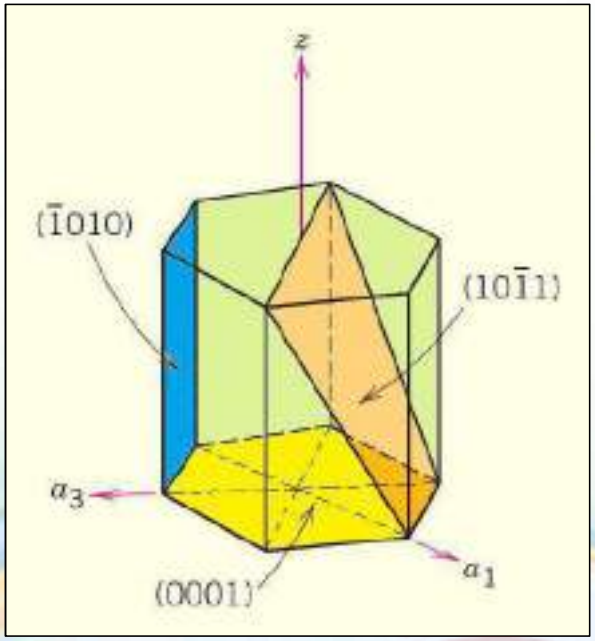
HCP Crystallographic Planes

- In hexagonal unit cells the same idea is used:

Example 3

	a_1	a_2	a_3	c
Intercepts	1	∞	-1	1
Reciprocals	1 1	1/∞ 0	-1 -1	1 1
Reduction	1	0	-1	1

Miller-Bravais Indices: $(1\ 0\ \bar{1}\ 1)$



(*) for BCC linear density in the main diagonal is the maximum

Linear Density

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

عدد الذرات المركزية على الوحدة الطول في الاتجاه المعين !! (مركز الذرة)

or how many diameter

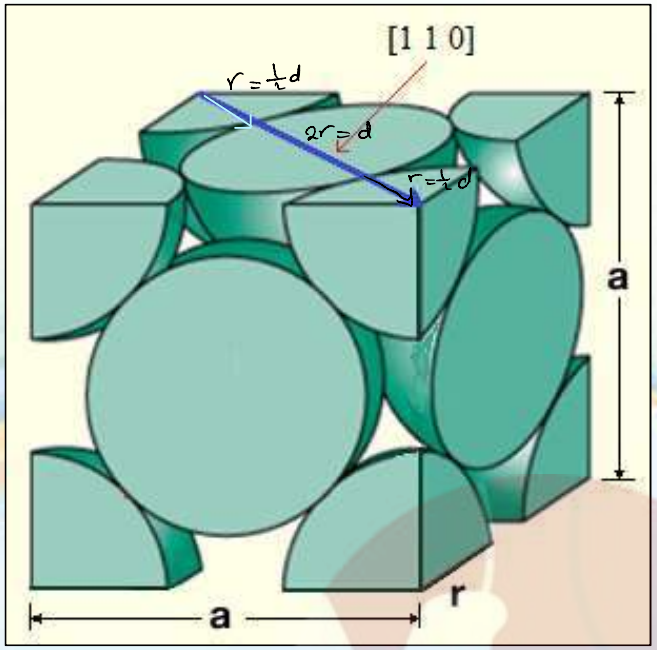
$= \frac{1}{2}d + \frac{1}{2}d + d$

$= 2d$

concentration of atoms per length (how many atoms exist in this length)

Example:

Calculate the linear density of Al in [1 1 0] direction. Al atomic radius = 0.143 nm



We know:

- Number of atoms centered = 2
- Unit length of direction vector = 4r

$$LD = \frac{2}{4 \times 0.143} = 3.4965\ nm^{-1}$$

$2d = 4r$

$d = 2r$

Radar ask & believe & recieve

Linear density

↳ $\frac{\text{number of atoms centered on unit length of direction vector}}{}$

لـ عدد الـ radius مضروب بـ 2 radius.

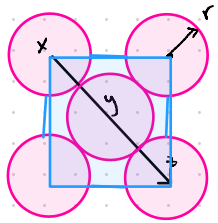
diameters لجعل كم عدد الـ
إلي بمر في خط سهم الـ
Direction
و منه مركز الدائرة

* يعني بالمثال إلي بالسابق إلي قبل ، عندنا زي ربع دائرة لكن فيها one radius و في فيها
بين في $2r$ و في دائرة كاملة بـ $2r$
العدد كامل = $4r$ ← تمثل unit length of direction vector
أما عدد الذرات بـ 2

⊛ أول إشي لازم أحدد الـ Direction وأركز السهم صح قبل ما أبدا
أطبق الـ linear Density .

planar density

$= \frac{\text{number of atoms centered on}}{\text{Area of the plane}}$



⊛ for calculations atoms are regarded as circles (Not a spheres!!)

⊛ بتحدد شكل الـ plane داخل الـ Building Block
بعدين بزرع شكل الـ 2D اللي plane جاد ديحتوي
على الذرات الداخلة في عشانه نحسب الـ Density
اضطر به .

ask believe & recieve

(*) one complete cross sectional area = one circle

Planar Density

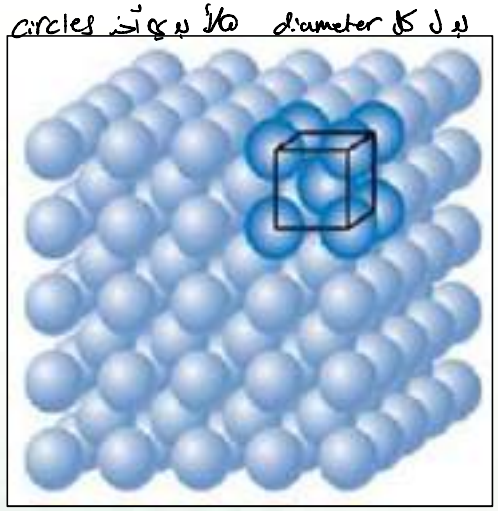
=> number of atoms exist in one cross sectional area

Example:

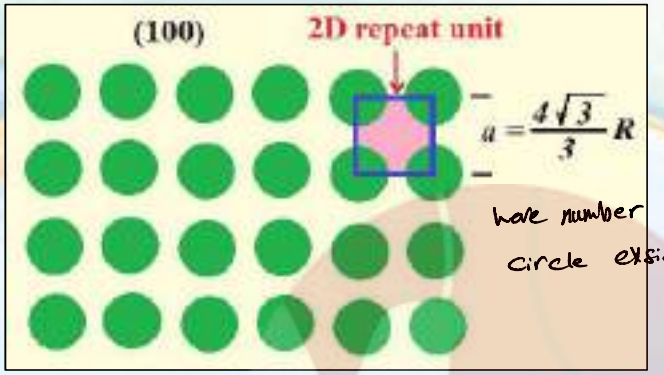
Calculate the Planar density of (1 0 0) Iron.

At T 912 oC iron has the BCC structure.

- Radius of iron R = 0.1241 nm
- Number of atoms in the plane = 1
- Area of plane = a^2



top view



$$Plamar\ Density = \frac{Number\ of\ atoms\ in\ the\ plane}{Area\ of\ the\ plane}$$

$$Plamar\ Density = \frac{1}{a^2} = \frac{1}{\left(\frac{4\sqrt{3}}{3}R\right)^2}$$

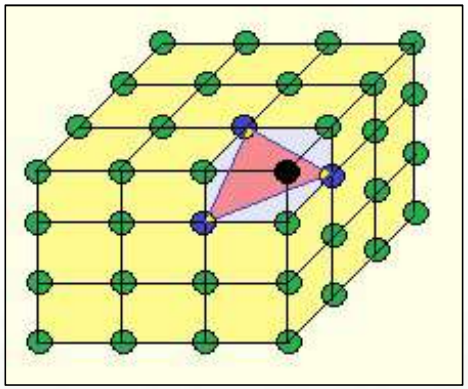
$$12.1\ \frac{atoms}{nm^2} = 1.2 \times 10^{19}\ \frac{atoms}{m^2}$$

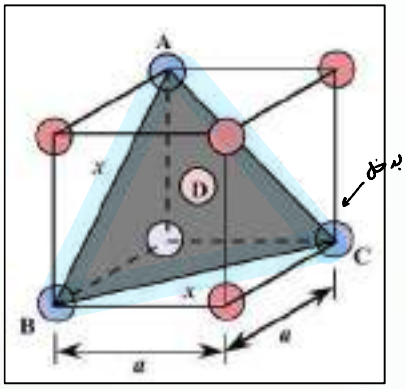
Radar ask & believe & recieve

Planar Density => how many circles exists / area

Excersise:

Calculate the planar density of (1 1 1) iron.



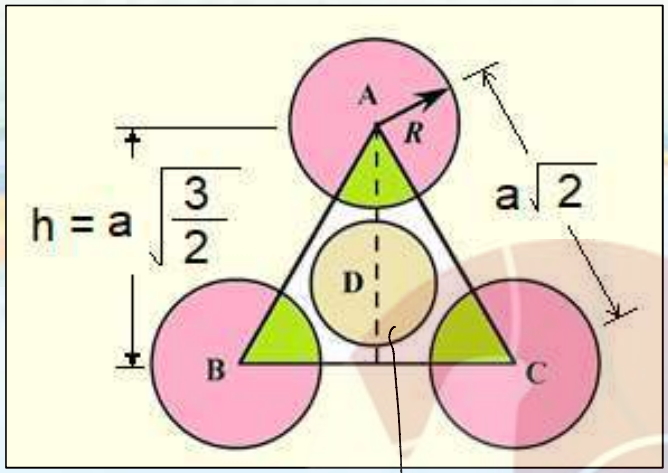


- *Radius of iron R = 0.1241 nm*
- *Number of atoms in the plane = 0.5*
- *Area of plane* $= \frac{\sqrt{3}}{2}a^2$

$$= \frac{\sqrt{3}}{2}\left(\frac{4}{\sqrt{3}}R\right)^2 = \frac{8}{\sqrt{3}}R^2$$

$$Plamar\ Density = \frac{0.5}{area} = \frac{0.5}{\frac{8}{\sqrt{3}}R^2}$$

$$= 0.703 \times 10^{19}\ \frac{atoms}{m^2}$$



هاد مو داخل لأنه حدود ال plane ما مرّت فيه

لو كانت مثلاً fcc وال plane بيمرّ بال face diagonal

لازم ال atoms هاد بالحساب بيضاعفوله 8 لأنه حدوده ما مرّت فيه.

Designating Lattice Planes

Why are planes in a lattice important?

A. Determining crystal structure:

- **Diffraction methods** measure the distance between parallel lattice planes of atoms. This information is used to determine the lattice parameters in a crystal.
- Diffraction methods also measure the angles between lattice planes.

B. Plastic deformation

- **Plastic deformation** in metals occurs by the slip of atoms past each other in the crystal.
- This slip tends to occur preferentially along specific crystal-dependent planes.

B. Transport Properties

In certain materials, atomic structure in some planes causes the transport of electrons and/or heat to be particularly rapid in that plane, and relatively slow in other planes.

Example:

Graphite: heat conduction is more in sp^2-bonded plane.

adar
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Chapter 4

IMPERFECTIONS IN SOLIDS

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Fall Semester 2022
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Outline

- What are the solidification mechanisms?
- What types of defects arise in solids?
- Can the number and type of defects be varied and controlled?
- How do defects affect material properties?
- Are defects undesirable?

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Solidification

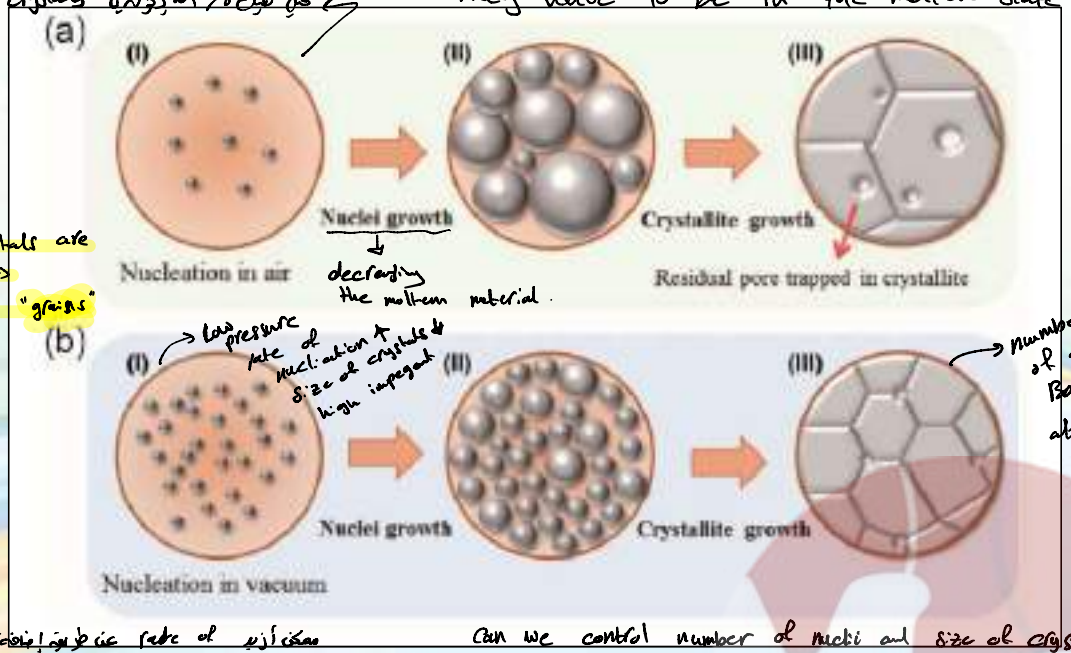
=> we'll get a homogenous mixture (distribution of Solute (minor) in the Solvent (major))

- **Start with a molten material – all liquid**

Result of casting of molten material:

1. Nuclei form.
2. Nuclei grow to form crystals – grain structure.
2. Crystals grow until they meet each other.

=> to mix any two or more metals They have to be in the molten State (above their Tm)



crystals

decreasing the molten material.

⊛ if the crystals are very small => They called "grains"

low pressure rate of nucleation ↑ Size of crystals ↓ high impegnat

number of grain Boundaries ↑ at lower pressure.

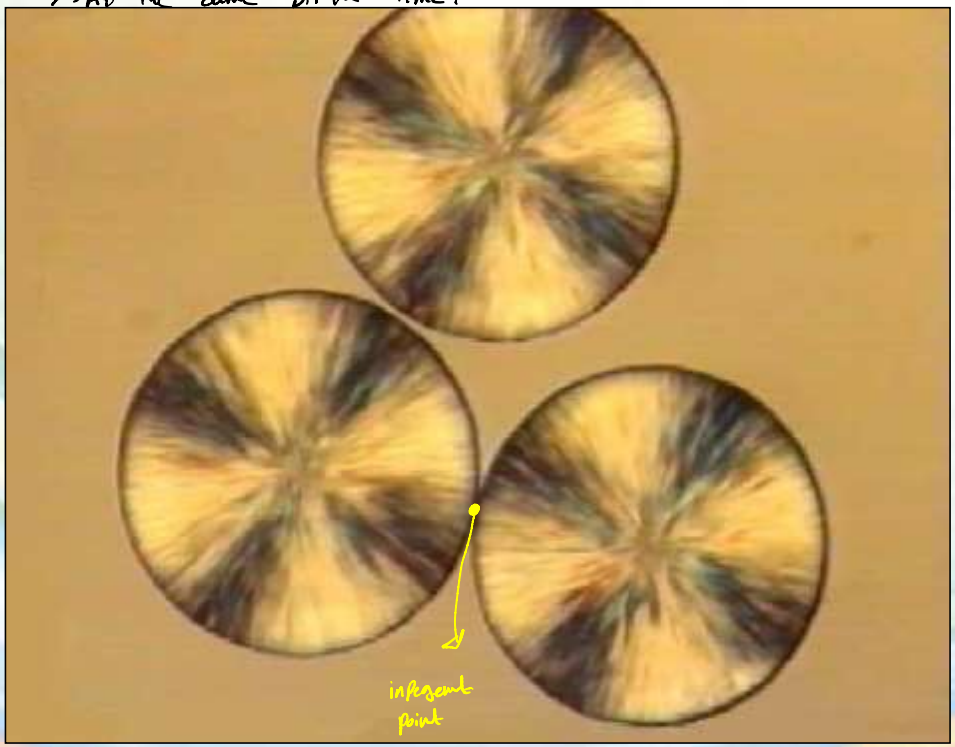
(adding) rate of nucleation

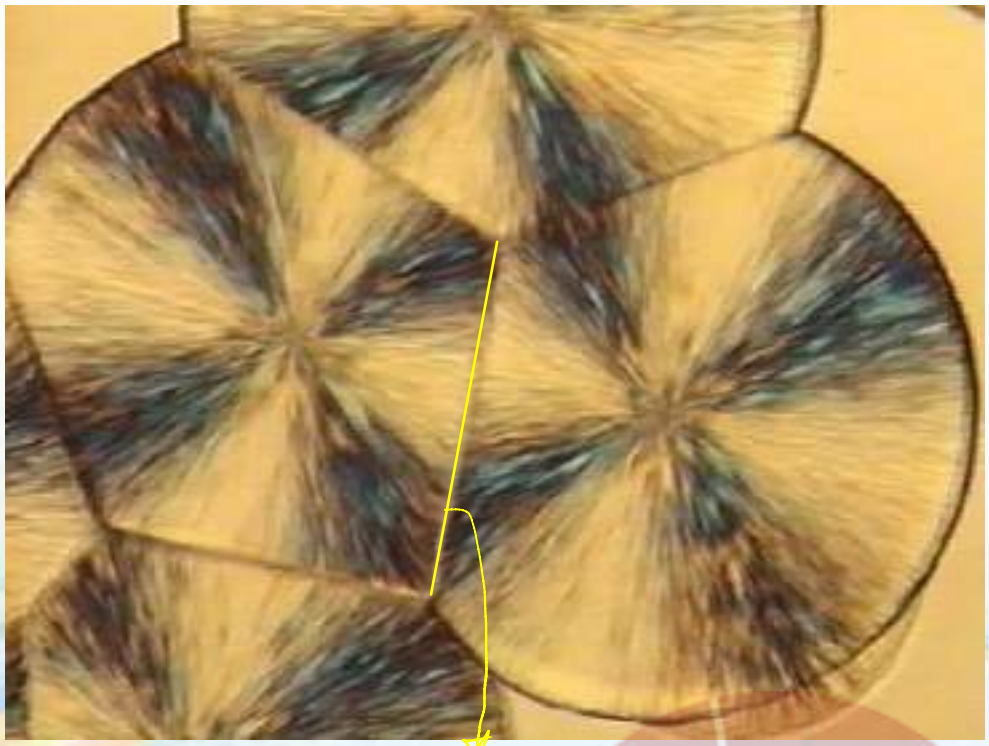
Can we control number of nuclei and size of crystals ?

yes!!

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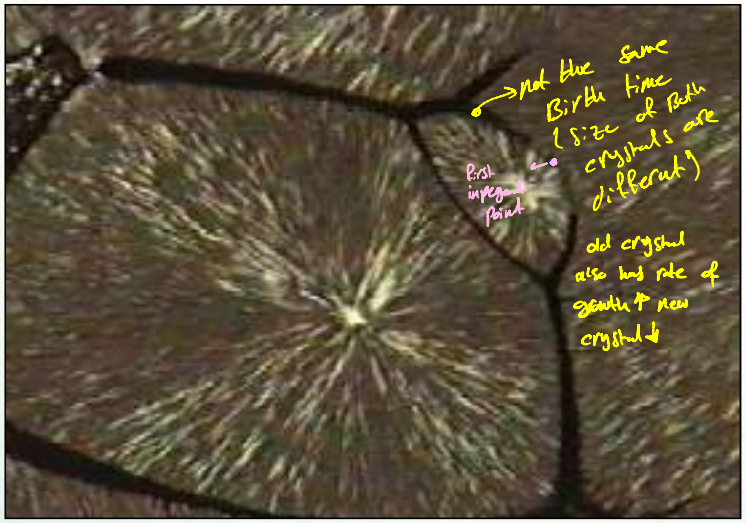
→ At the same birth time.

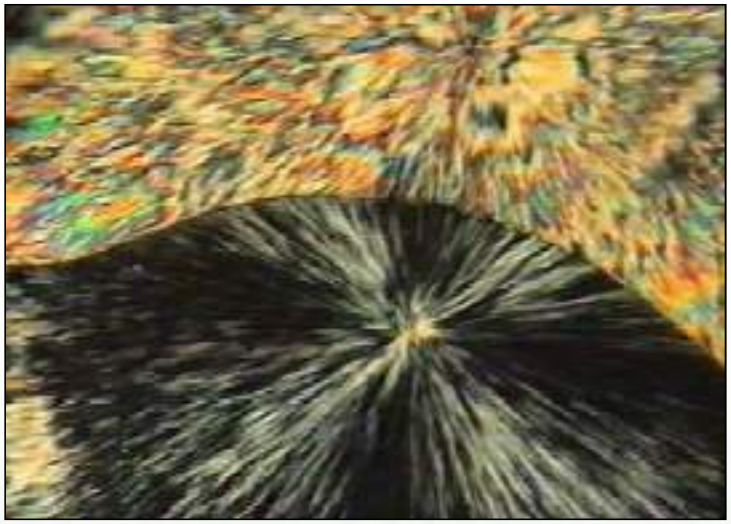


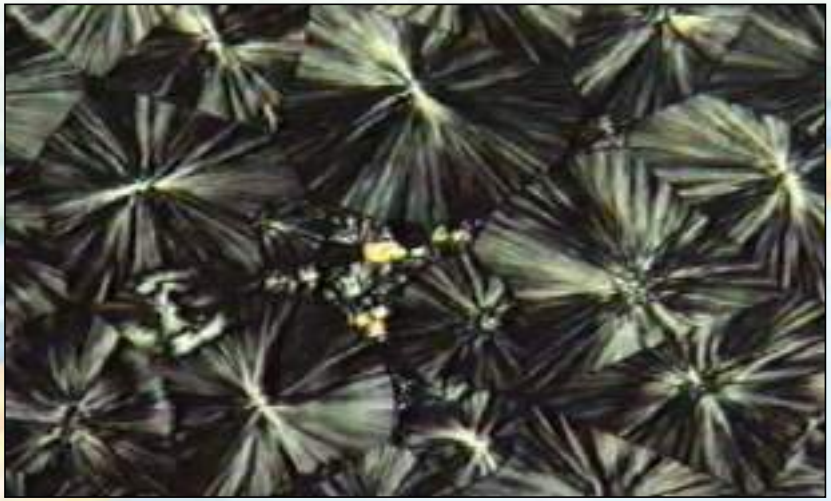


grain Boundary is straight line because they have same rate of growth + type of crystal + birth time are the same.

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Failure occurs at the grain boundaries
↳ Also called "Stress Concentration Area"

Crystalline Structure

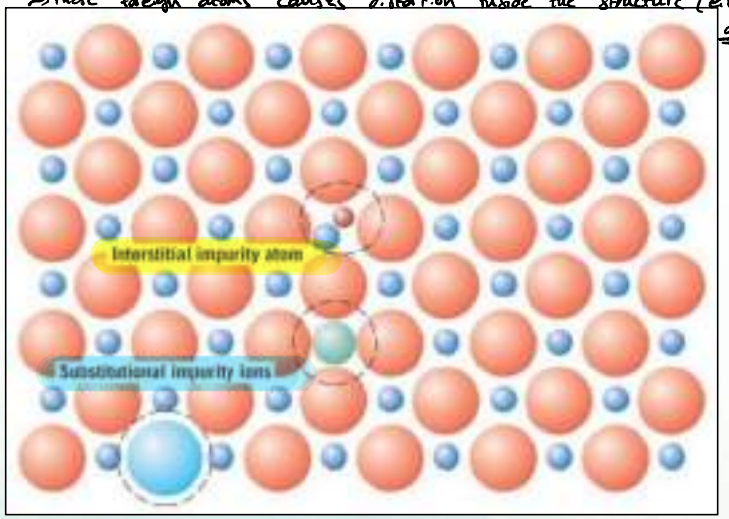
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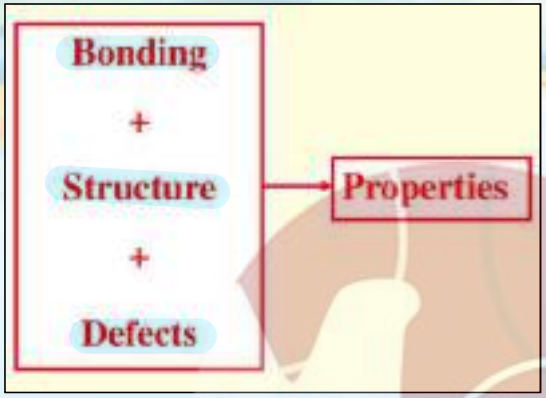
Experiment 2
Hot Ice Sea Urchin

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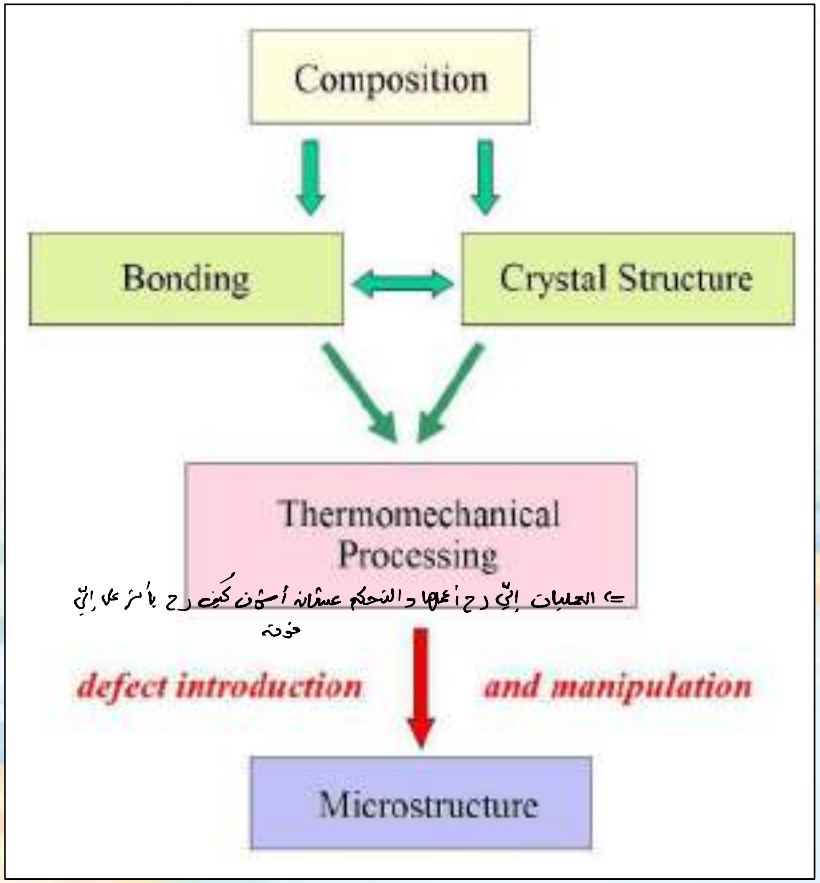
Imperfections in Solids

- There is no such thing as a perfect crystal.
  - ✓ What are these imperfections?
  - ✓ Why are they important?
- Many of the important properties of materials are due to the presence of imperfections.
- Defects have a profound impact on the macroscopic properties of materials.
  - ✓ Semiconducting properties
  - ✓ Yield stress
  - ✓ Fracture strength
  - ✓ Electrical conductivity



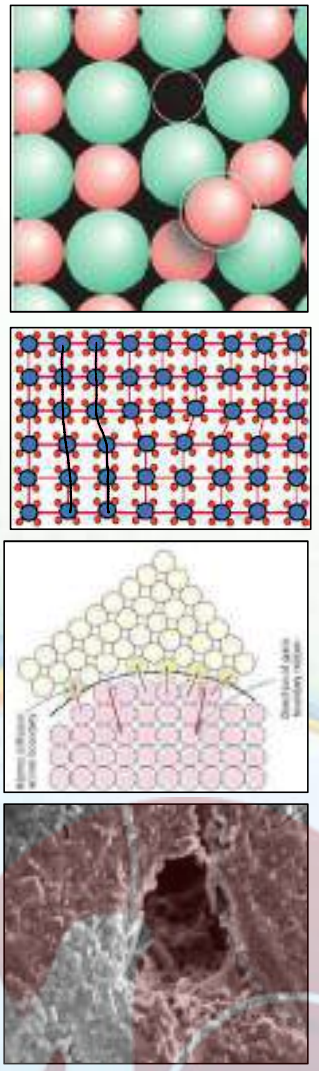


- *The processing determines the defects imperfections*



Types of Imperfections

1. **Point defects:** atoms missing or in irregular places in the lattice
   - Vacancies
   - Interstitials (space that intervenes between things).
   - Impurities, weight and atomic composition
2. **Line defects:** groups of atoms in Irregular Positions: edge dislocations and screw dislocations
3. **Area defects:** the interfaces between homogeneous regions of the material
   - Grain boundaries
4. **Bulk or Volume defects:**
   - Pores
   - Cracks

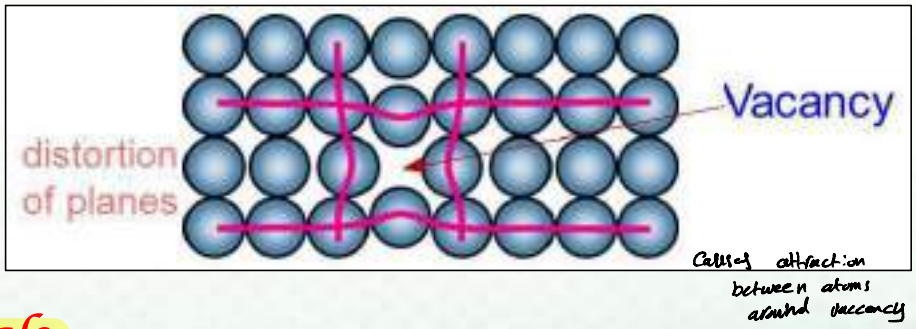


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Point Defects

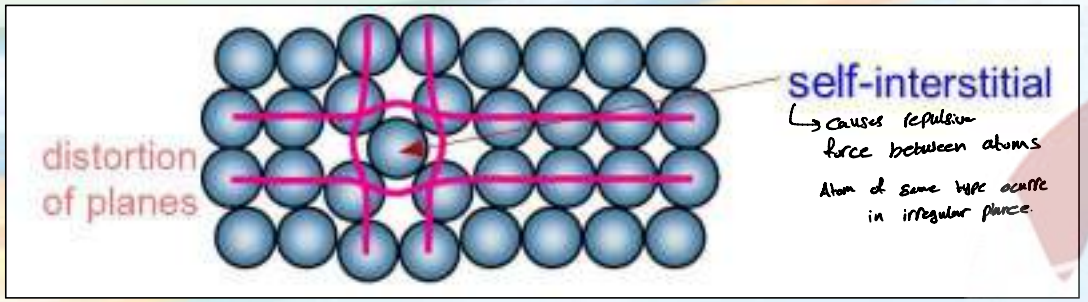
➢ Vacancies

This figure shows a vacant atomic sites in a structure.



➢ Self-Interstitials

"Extra" atoms positioned between atomic sites.



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How many vacancies are there?

- The equilibrium number of vacancies formed as a result of thermal vibrations may be calculated from thermodynamics:

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

Where:

How many vacancy at any T?
vacancy # @ T #

N_v: Number defects

N_s: Number of potential defect sites → number of atoms in the cm^3 (chapter 2)

K: Boltzmann's constant; 1.38×10^{-23} J/atom-K or 8.62×10^{-5} eV/atom-K

T: Temperature

Q_v: Activation energy

Each lattice site is a potential vacancy site

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Example:

Estimate the number of vacancies in Cu at room temperature.

$$N_v = N_s exp\left(\frac{-Q_v}{k_B T}\right)$$ → if Q_v in eV ⇒ k must be on eV ⇒

- *The Boltzmann's constant* $k_B = 1.38\times10^{-23}$ *J/atom-K or* 8.62×10^{-5} *eV/atom-K*
- *The temperature in Kelvin* $T = 27\ ^oC + 273 = 300\ K$
- $k_B T = 300\ K \times 8.62 \times 10^{-5}\ eV/K = 0.02586\ eV$
- *The energy for vacancy formation* $Q_v = 0.9\ eV/atom$
- *The number of regular lattice sites* $N_s = \frac{N_A \rho}{A_{Cu}}$
- $N_A = 6.023 \times 10^{23}$ *atoms/mol*
- $\rho = 8.4\ g/cm^3$
- $A_{Cu} = 63.5\ g/mol$

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$$N_s = \frac{6.023 \times 10^{23}\ atoms/mol \times 8.4\ g/cm^3}{63.5\ g/mol} = 7.967 \times 10^{22}\ \frac{atoms}{cm^3}$$

$$N_v = 7.967 \times 10^{22}\ \frac{atoms}{cm^3}\ exp\left(\frac{-0.9\ eV/atom}{0.02586\ eV/atom}\right)$$

$$= 6.12 \times 10^{7}\ \frac{vacancies}{cm^3}$$

Temperature °C	N_v	Weight %
27	6.12×10^{7}	$7.68\ 10^{-14}$
40	259.67×10^{7}	$3.26\ 10^{-13}$
100	5.556×10^{10}	$6.97\ 10^{-11}$
400	1.458×10^{16}	$1.83\ 10^{-5}$
600	5.096×10^{17}	0.00064
900	1.086×10^{19}	0.01363
1700	4.01×10^{20}	0.5032

ذرات النحاس مؤثر على مغادرة ←

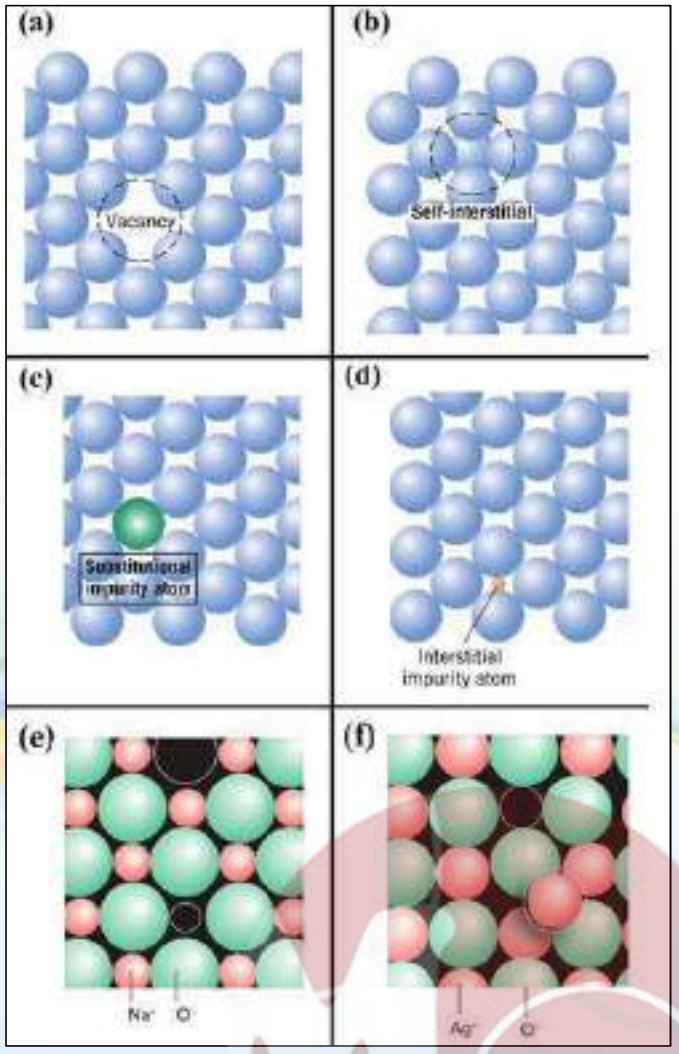
Thermal vibration frequency تسبب زيادة الذرات

فانذكر الروابط و مغادر الذرات مكانها (حد ما يصير كله (molten)

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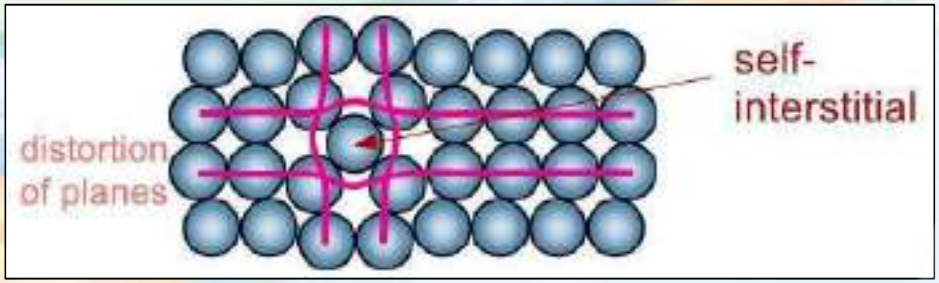
Other point defects: self-interstitials, impurities

- Schematic representation of different point defects:
  - (a) Vacancy
  - (b) Self-interstitial
  - (c) Substitutional impurities
  - (d) Interstitial impurity



Self-interstitials

- Self-interstitials in metals introduce large distortions in the surrounding lattice .
- The energy of self-interstitial formation is ~ 3 times larger as compared to vacancies ($Q_i \sim 3 \times Q_v$).
- Equilibrium concentration of self-interstitials is very low (less than one self-interstitial per cm^3 at room T).



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Impurities

- **Impurities** - atoms which are different from the host.
  - ✓ All real solids are impure.
  - ✓ Very pure metals 99.9999% - one impurity per 10^6 atoms.
  - ✓ May be intentional or unintentional.
    - to change the properties of the material.
    - Such as Analytical grains
- **Examples**:
  - ✓ Carbon added in small amounts to iron makes steel, which is stronger than pure iron.
  - ✓ Boron added to silicon change its electrical properties.
- **Alloys**: deliberate mixtures of metals.
- Example: sterling silver is 92.5% silver – 7.5% copper alloy. Stronger than pure silver.

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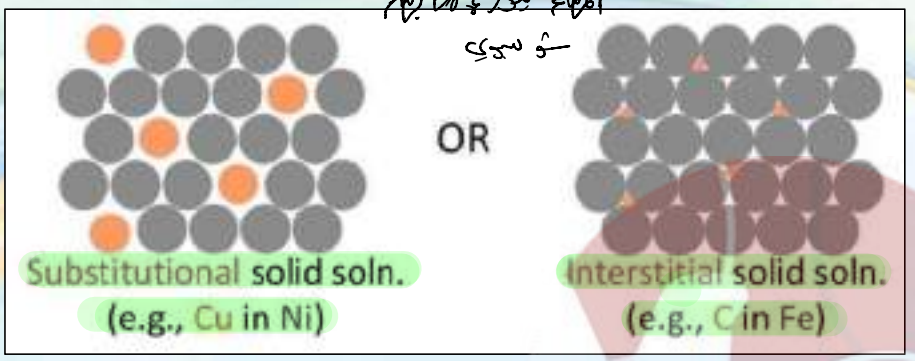
Solid Solutions

- Solid solutions are made of a host (the solvent or matrix) which dissolves the minor component (solute).
- The ability to dissolve is called solubility.
- Solvent: in an alloy, the element or compound present in greater amount.
- Solute: in an alloy, the element or compound present in lesser amount.

when we add an impurities we expect to have only these type of solutions

1. Solid Solution

- ✓ Homogeneous
- ✓ Maintain crystal structure
- ✓ Contain randomly dispersed impurities (substitutional or interstitial)

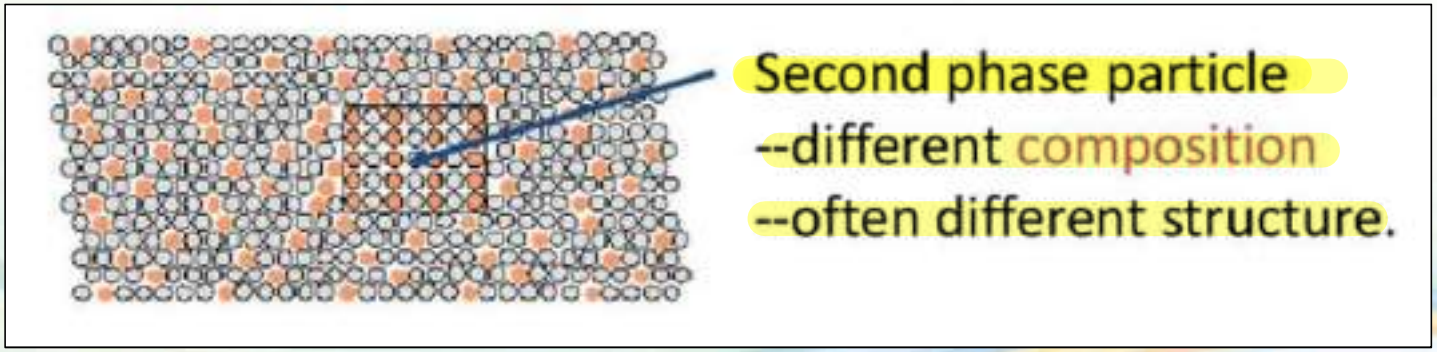


we don't want from the foreign atoms to arrange together

Solid Solutions ⇒ depends on Solubility !!

2. Second Phase:

As solute atoms are added, new compounds / structures are formed, or solute forms local precipitates.



- *Whether the addition of impurities results in formation of solid solution or second phase depends on the nature of the impurities, their concentration and temperature, pressure…*

Substitutional Solid Solutions

إذا تحققت الـ Hume Rothery في Substitutional Solid Solution.

Factors for high solubility: (Hume – Rothery rule)

- **Atomic size factor** - atoms need to "fit" solute and solvent atomic radii should be within ~ ±15%. If size difference of elements are greater than 15%, the lattice distortions (local lattice strain) are too big and solid-solution will not be favored.

$$DR\% = \frac{r_{solute} - r_{solvent}}{r_{solvent}} \times 100\%$$

- **Crystal structures:** like elemental crystal structure are better. For appreciable solubility, the crystal structure for metals must be the same, i.e. solute and solvent should be the same.

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Substitutional Solid Solutions

- **Electronegativity:** $DE \sim 0$ favors solid-solution.

$$DR\% = \frac{E_{solute} - E_{solvent}}{E_{solvent}} \times 100\%$$

The more electropositive one element and the more electronegative the other, then intermetallic compounds are more likely.

they must have two low electronegative (or +ve)
or high electronegative (or +ve)

- **Valence:** Generally more solute goes into solution when it has **higher valency** than solvent.

Higher in lower alright. Lower in higher, it's a fight.

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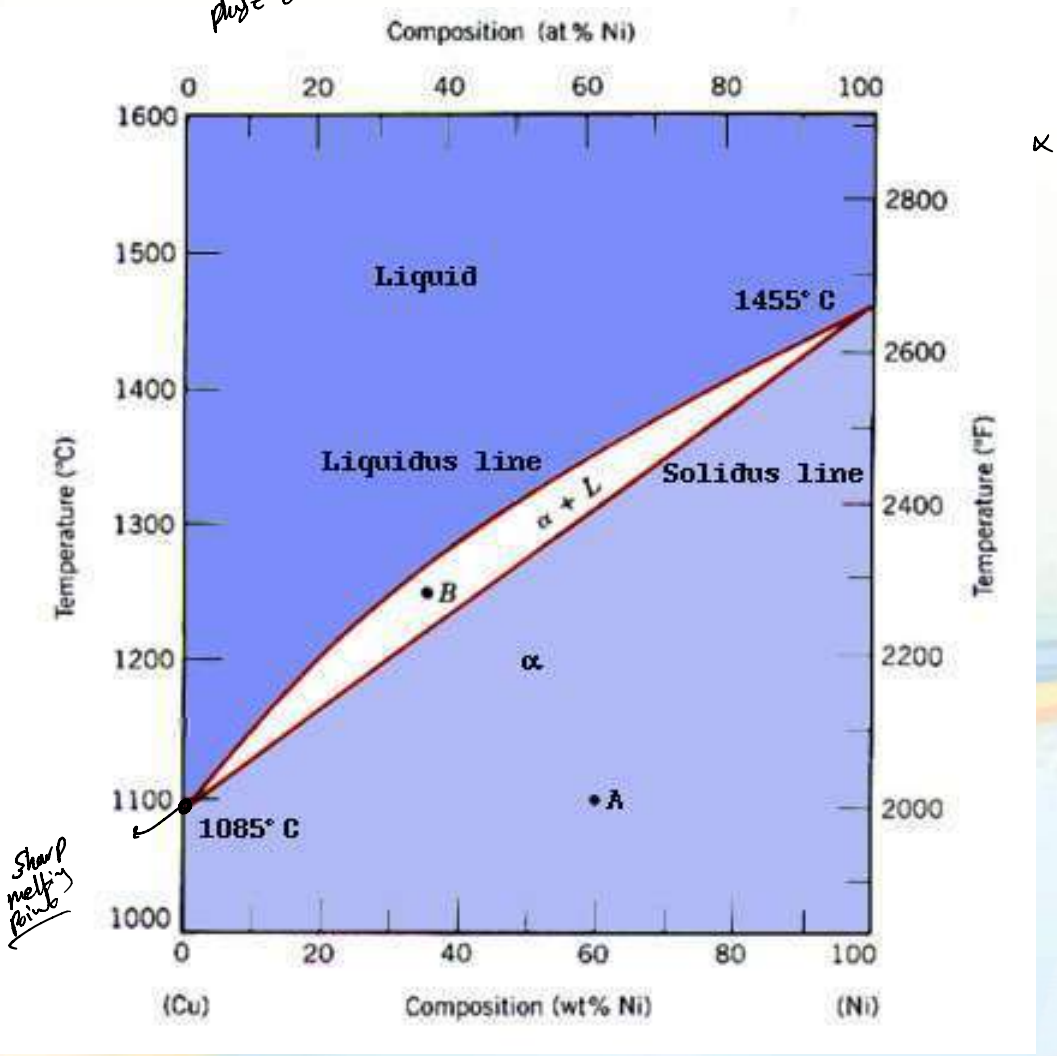
Example

Is solid-solution favorable, or not for Cu-Ni alloys?

- ✓ Rule 1: $r_{Cu} = 0.1278$ nm and $r_{Ni} = 0.1246$ nm
  DR% = (0.1246-0.1278)/0.1278*100% = 2.5% (Favorable)
- ✓ Rule 2: Ni and Cu have the FCC crystal structure (Favorable)
- ✓ Rule 3: $E_{Cu} = 1.9$ and $E_{Ni} = 1.8$. Thus,
  DE% = (1.8-1.9)/1.9*100% = -5.2 % (Favorable)
- ✓ Rule 4: Valency of Ni and Cu are both +2. (Favorable)

➢ Expect Ni and Cu forms S.S. over wide composition range

Isomephous phase diagram



Sharp melting point

لو أخذت سبيكة أحد أطرافها (Cu: %20, Ni: %80)

4 factors of hume rothery rule are applicable

we have an unlimited solubility and we can do with of who is the solvent (most) and who is the solute

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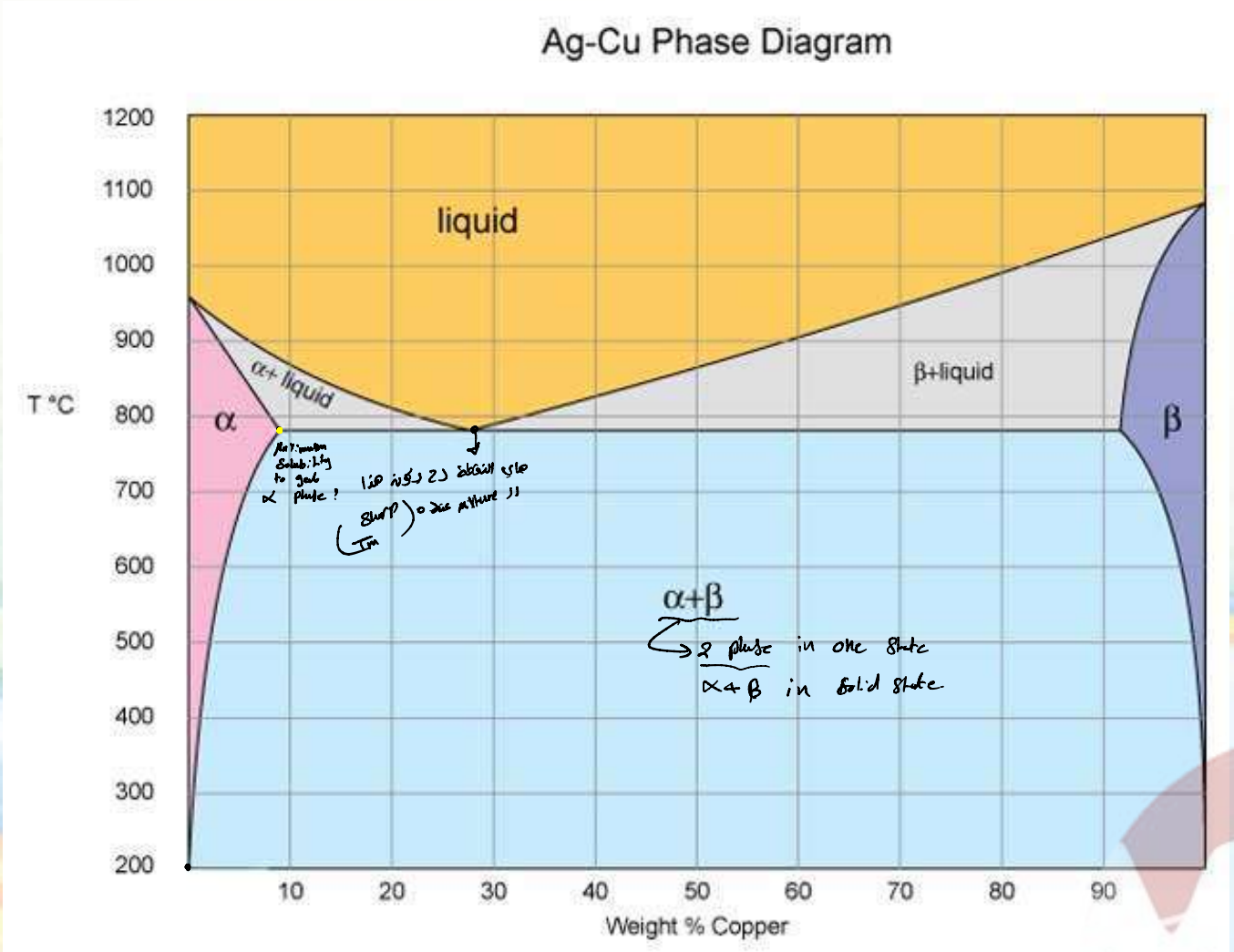
Example

Is solid-solution favorable, or not for Cu-Ag alloys?

- ✓ *Rule 1:* $r_{Cu} = 0.1278$ nm and $r_{Ni} = 0.1445$ nm
  $DR\% = (0.1445-0.1278)/0.1278*100\% = 13\%$ *(Favorable)*
- ✓ *Rule 2: Ag and Cu have the FCC crystal structure* *(Favorable)*
- ✓ *Rule 3:* $E_{Cu} = 1.9$ and $E_{Ni} = 1.9$. *Thus,*
  $DE\% = 0\%$ *(Favorable)*
- ✓ *Rule 4: Valency of Cu is +2 and Ag is +1* *(Not favorable)*

- ➢ *Expect Ag and Cu have limited solubility.*
- ➢ *In fact, the Cu-Ag phase diagram shows that a solubility of only 18% Ag can be achieved at high T in the Cu-rich alloys.*

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Ag-Cu Phase Diagram
liquid
α+ liquid
β+liquid
α
β
α+β
T °C
1200
1100
1000
900
800
700
600
500
400
300
200
10
20
30
40
50
60
70
80
90
Weight % Copper

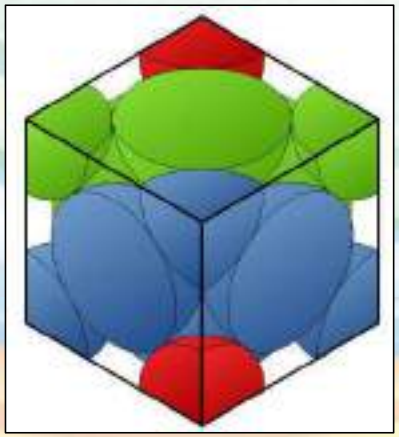
Solid Solutions

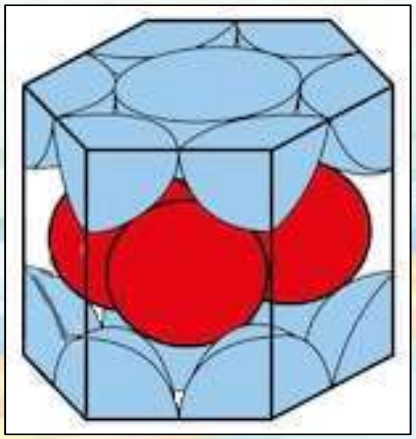
Application of Hume – Rothery rules – Solid Solutions.

1. Would you predict more Al or Ag to dissolve in Zn?

2. More than Zn or Al in Cu?

Al and Ag *Zn*





Element	Atomic Radius (nm)	Crystal Structure	Electro-nega-tivity	Valence
Cu	0.1278	FCC	1.9	+2
C	0.071			
H	0.046			
O	0.060			
Ag	0.1445	FCC	1.9	+1
Al	0.1431	FCC	1.5	+3
Co	0.1253	HCP	1.8	+2
Cr	0.1249	BCC	1.6	+3
Fe	0.1241	BCC	1.8	+2
Ni	0.1246	FCC	1.8	+2
Pd	0.1376	FCC	2.2	+2
Zn	0.1332	HCP	1.6	+2

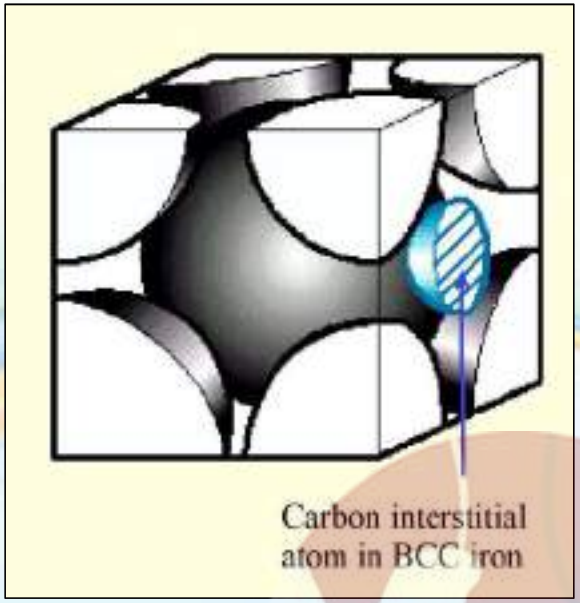
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Interstitial Solid Solutions

- Interstitial solid solution of C in α-Fe. The C atom is small enough to fit, after introducing some strain into the BCC lattice.

Factors for high solubility:

- For FCC, BCC, HCP structures the voids (or interstices) between the host atoms are relatively small, atomic radius of solute should be significantly less than solvent.
- Normally, max. solute concentration ≤ 10%, (2% for C-Fe)



Carbon interstitial atom in BCC iron

Composition / Concentration

Composition can be expressed in:

- **Weight percent**, useful when making the solution.
- **Atom percent**, useful when trying to understand the material at the atomic level.
- **Weight percent (wt %)**: weight of a particular element relative to the total alloy weight.
- For two-component system, concentration of element 1 in wt. % is

$$C_1 = \frac{m_1}{m_1 + m_2} \times 100$$

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Composition / Concentration

- **Atom percent (at %):** number of moles (atoms)) of a particular element relative to the total number of moles (atoms) in alloy.
- For two-component system, concentration of element 1 in at. % is:

$$C_1' = \frac{n_{m1}}{n_{m1} + n_{m2}} \times 100$$

where $n_{m1} = m'_1/A_1$

m'_1 is weight in grams of element 1.

A_1 is atomic weight of element 1.

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Composition Conversions

- Weight % to Atomic %

$$C_1' = \frac{C_1 A_2}{C_1 A_2 + C_2 A_1} \times 100$$

$$C_2' = \frac{C_2 A_1}{C_1 A_2 + C_2 A_1} \times 100$$

- Atomic % to Weight %

$$C_1 = \frac{C_1' A_1}{C_1' A_1 + C_2' A_2} \times 100$$

$$C_2 = \frac{C_2' A_2}{C_1' A_1 + C_2' A_2} \times 100$$

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Dislocations —Linear Defects

=> many of atoms in series causes this defect.

- Dislocations are very important in mechanical properties of material.
- Introduction/discovery of dislocations in 1934 by Taylor, Orowan and Polyani marked the beginning of understanding of mechanical properties of materials.

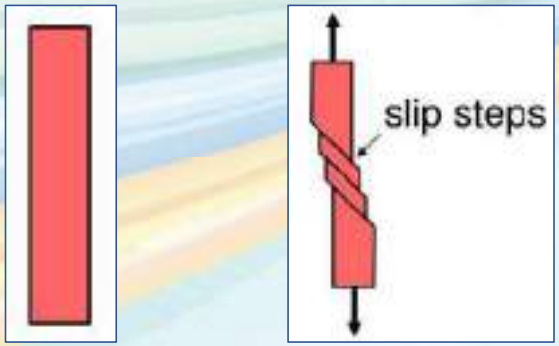
two types of linear defects
1) edge dislocation
2) screw dislocation
but in real life they are not shown alone and explicity => it is a mixture

- Dislocations are line defects.
- Slip between crystal planes result when dislocations move.

↳ displacement of atoms from their location to a new location (mainly in the lamina) Building block => because of this movement the bonding will break down and reformulate again

- Dislocations produce permanent (plastic) deformation.

Before deformation



After tensile elongation

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Dislocations —Linear Defects

- ✓ Are one-dimensional defects around which atoms are misaligned

- ➢ **Edge dislocation:**
  - ✓ Extra half-plane of atoms inserted in a crystal structure.
  - ✓ b perpendicular to dislocation line.

- ➢ **Screw dislocation:** => shear force
  - ✓ Spiral planar ramp resulting from shear deformation.
  - ✓ b parallel to dislocation line

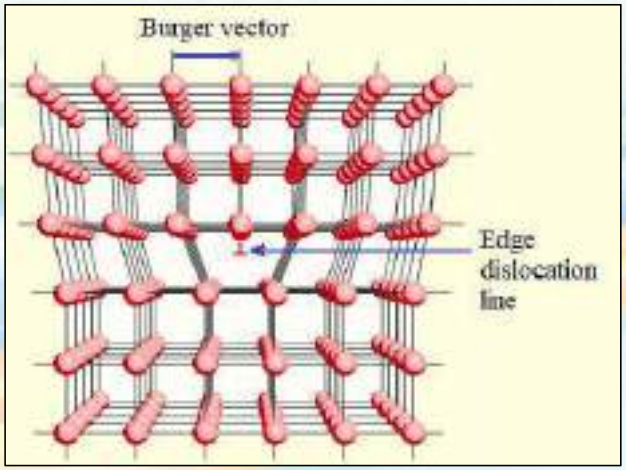
Burger's vector b: measure of lattice distortion.

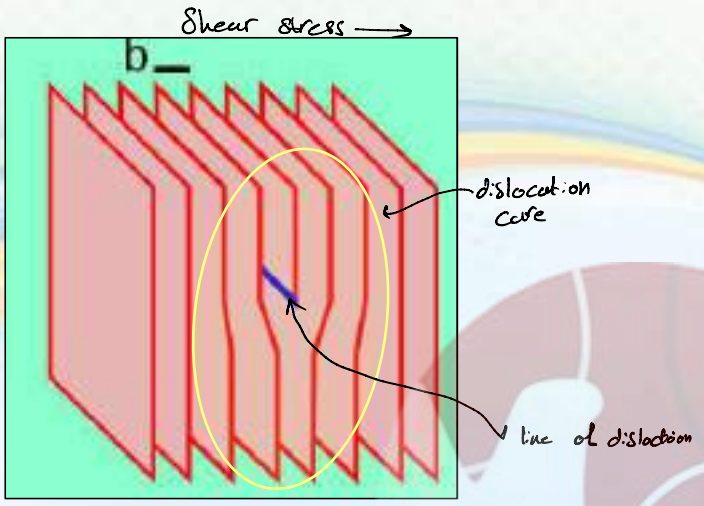
↳ by what unit does the lattice deformate (displaced from it's location to another one)

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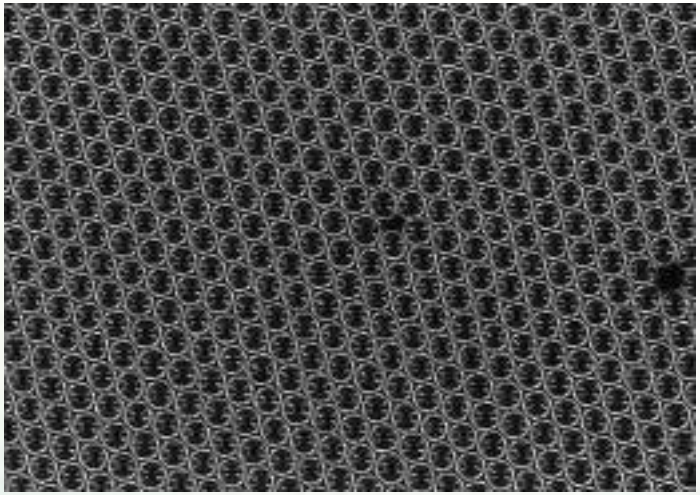
Edge dislocation

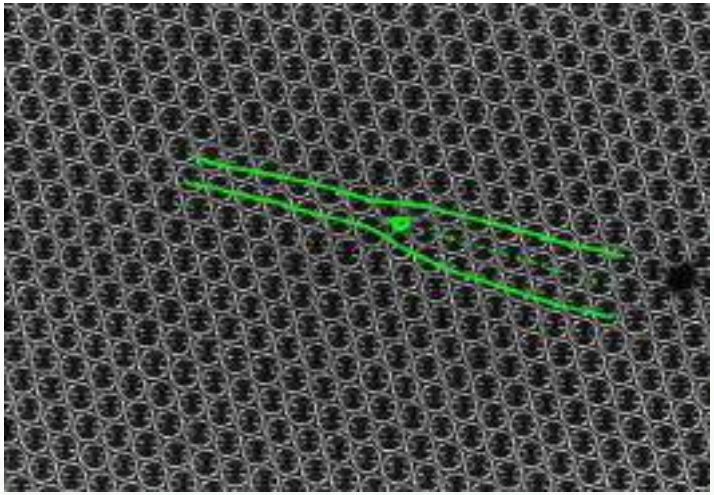
- Dislocations are linear defects: the interatomic bonds are significantly distorted only in the immediate vicinity of the dislocation line
- This area is called the dislocation core.
- Dislocations also create small elastic deformations of the lattice at large distances.

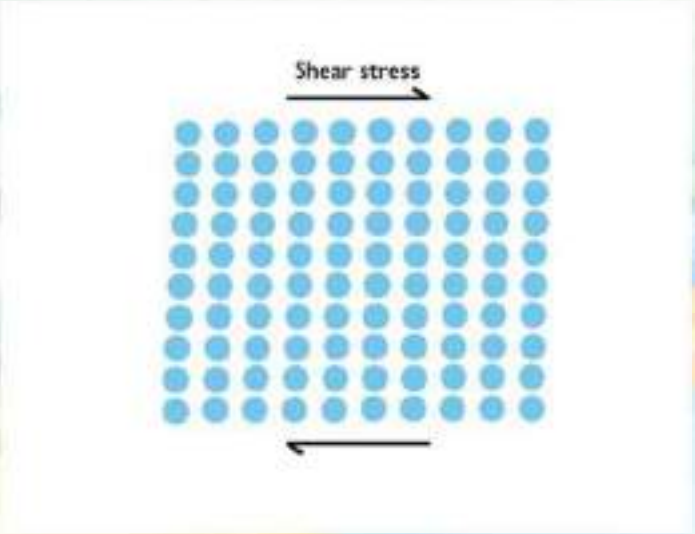




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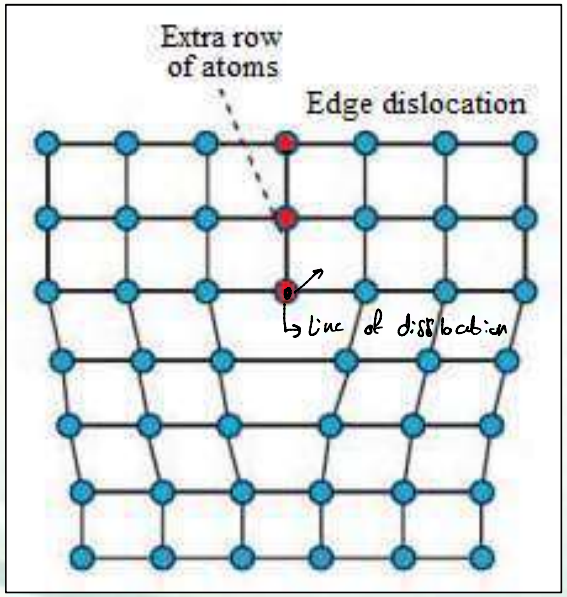
adar
ask :: believe & recieve

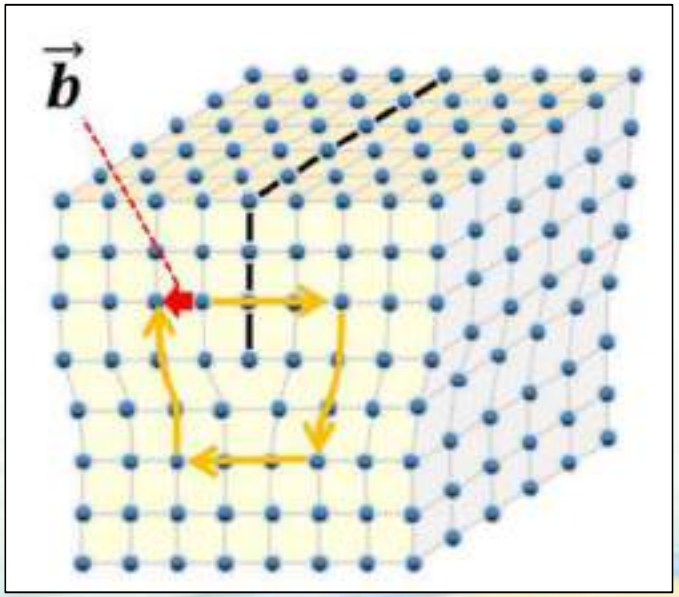
Motion of Edge Dislocation

- Dislocation motion requires the successive bumping of a half plane of atoms.
- Bonds across the slipping planes are broken and remade in succession
- To describe the size and the direction of the main lattice distortion caused by a dislocation we should introduce so-called Burgers vector b.
- To find the Burgers vector, we should make a circuit from atom to atom counting the same number of atomic distances in all directions.
- If the circuit encloses a dislocation it will not close.
- The vector that closes the loop is the Burgers vector b.

↳ how many units to close this circuit

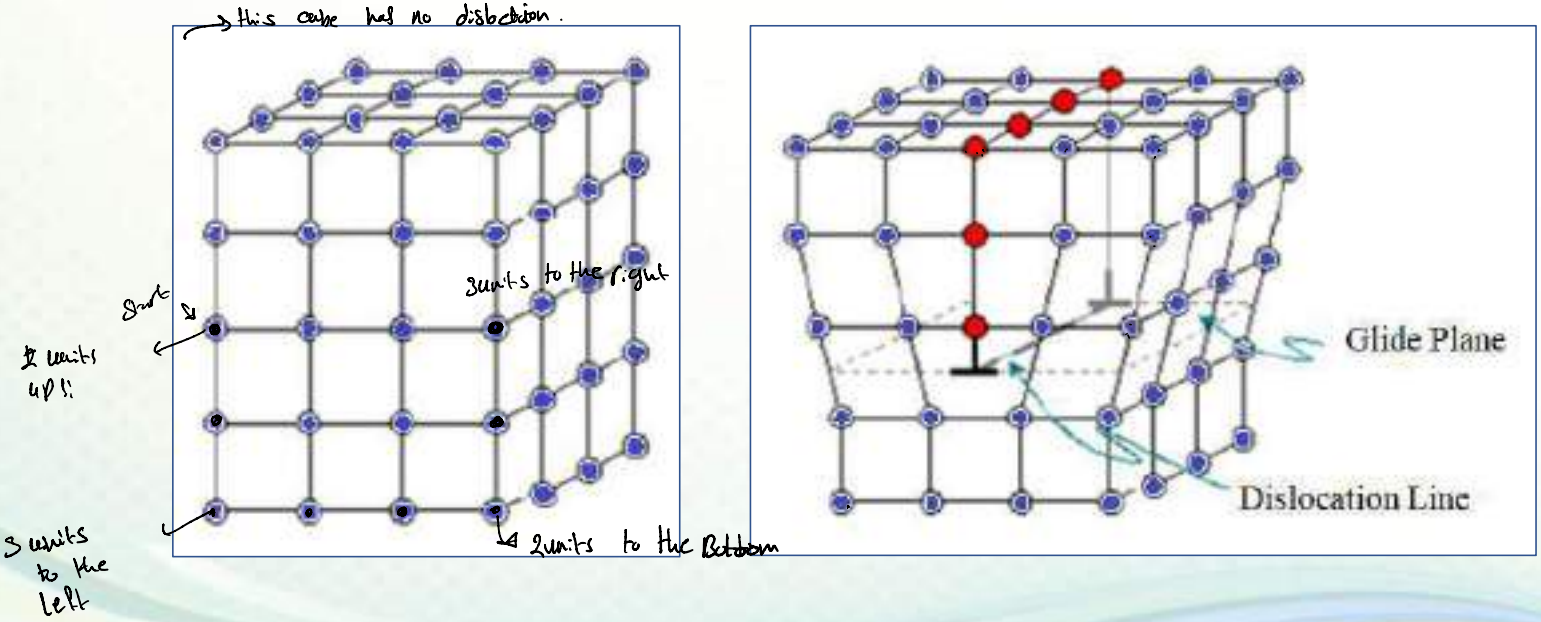
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- *Dislocations shown above have Burgers vector directed perpendicular to the dislocation line.*
- *These dislocations are called edge dislocations.*

Radar ask :: believe & recieve

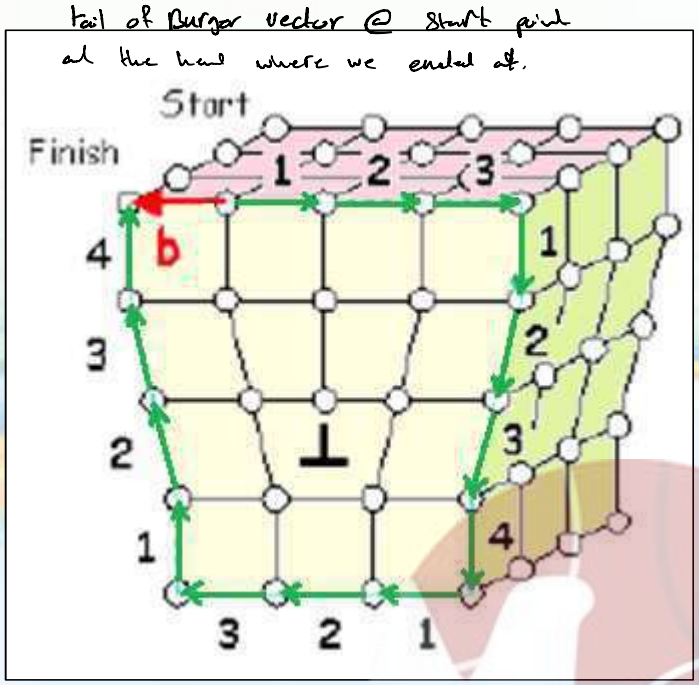


- *Introducing a dislocation into a crystal lattice by cramming in an extra half-plane.*
- *The dislocation line marks the edge of the half-plane. The inverted T symbol shows the location of the half-plane.*

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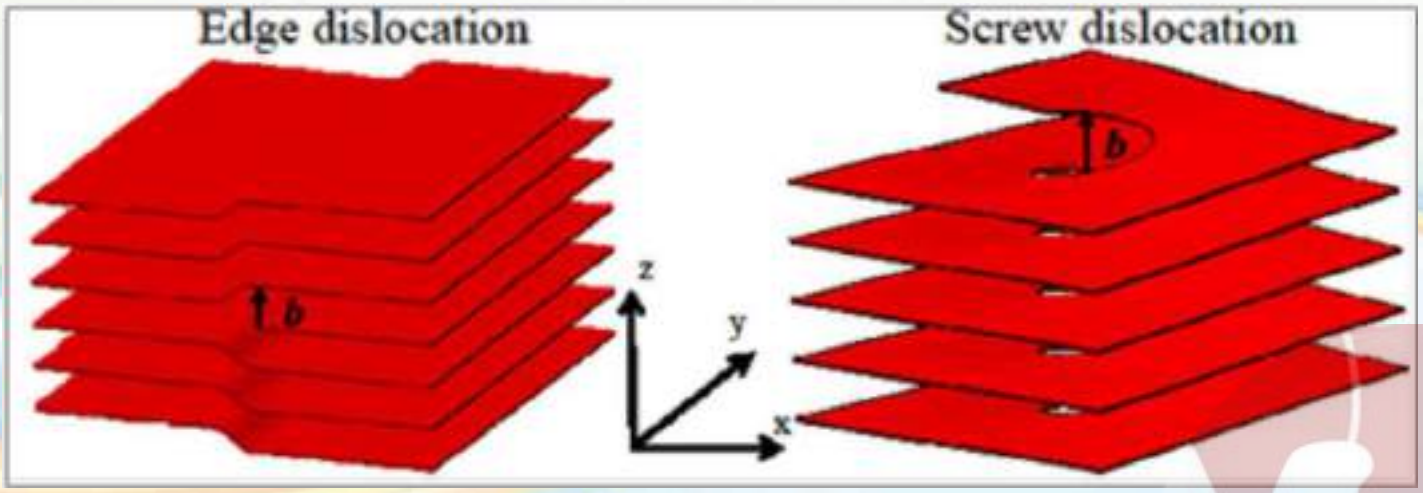
Burgers vector

- Start at some point, going clockwise around the dislocation and counting our steps so that we take the same number right as we took left, the same number down as we took up and so on.
- Once we have circled the dislocation and our steps match up, the Burgers vector is the vector which points from Start to Finish.

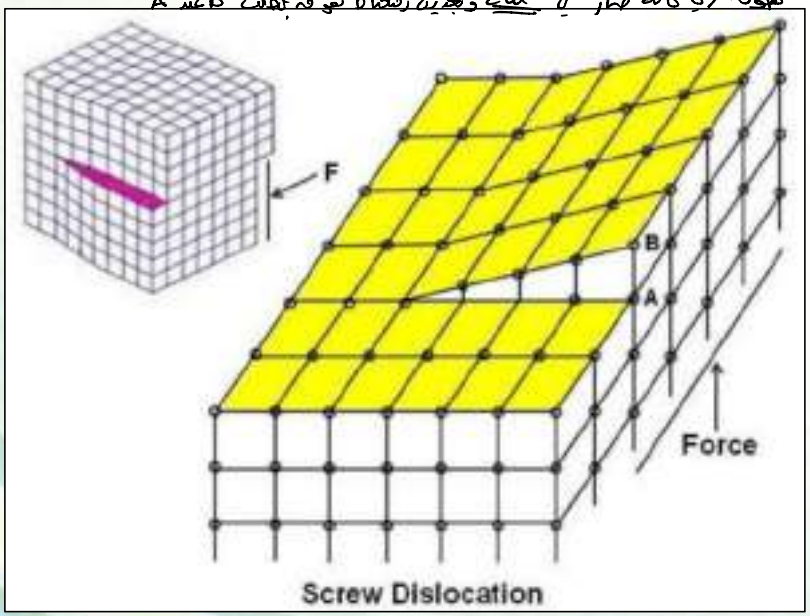


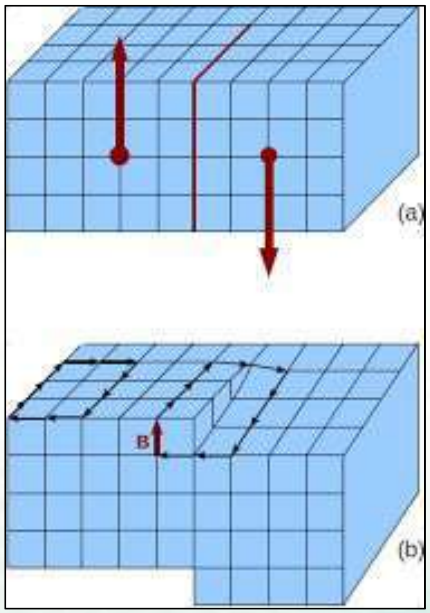
Screw dislocations

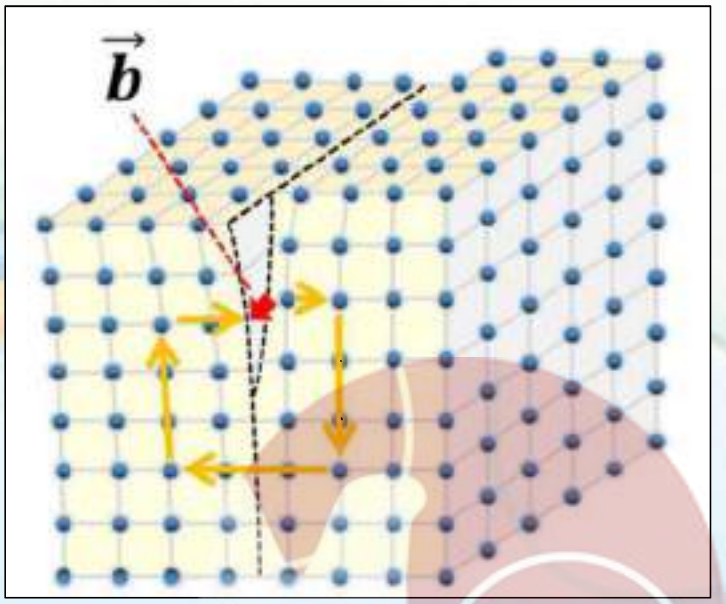
- Dislocations shown in previous slide are edge dislocations, have Burgers vector directed perpendicular to the dislocation line.
- There is a second basic type of dislocation, called screw dislocation



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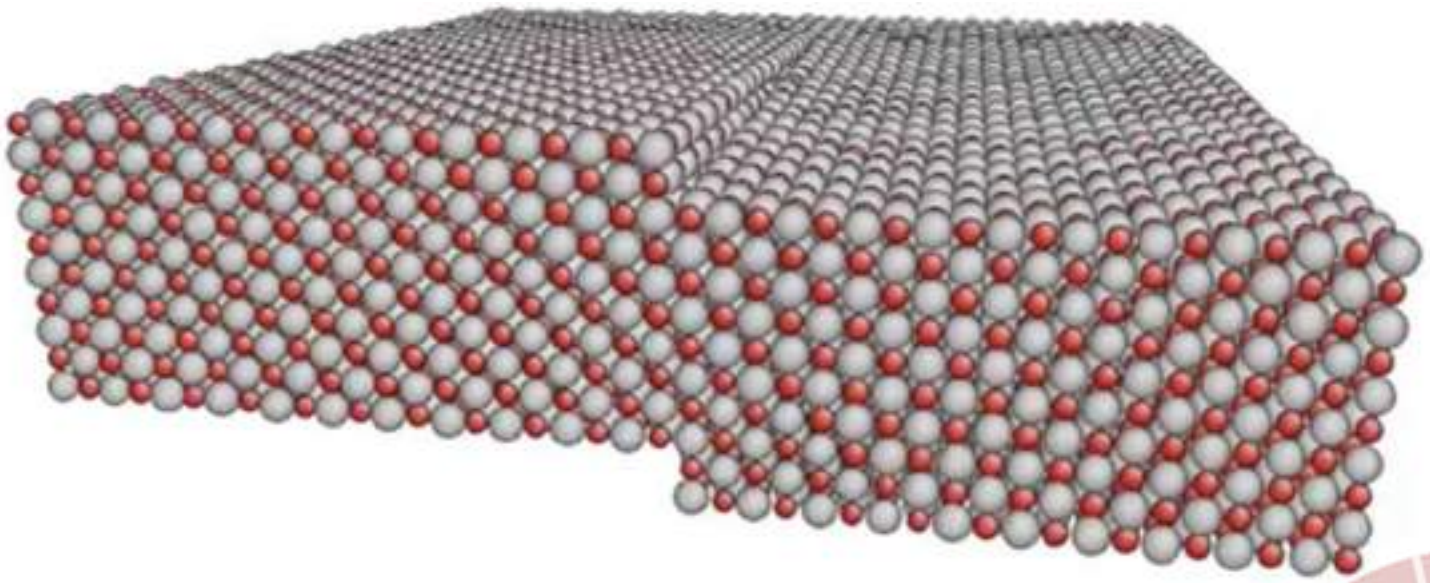




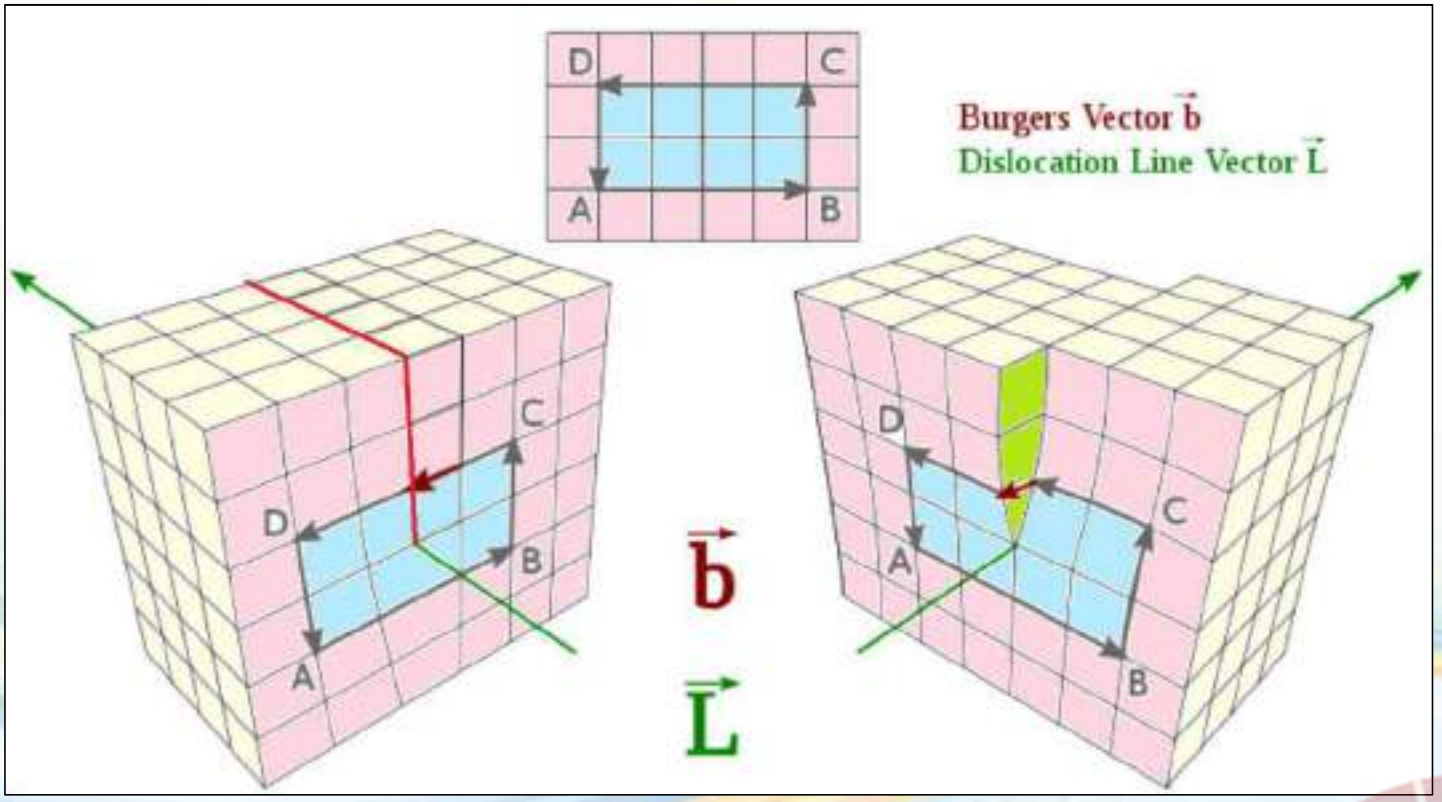


- *The screw dislocation is parallel to the direction in which the crystal is being displaced (Burgers vector is parallel to the dislocation line).*

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A screw dislocation is like a spiral staircase or a parking garage. The dislocation line is the axis of the helix.

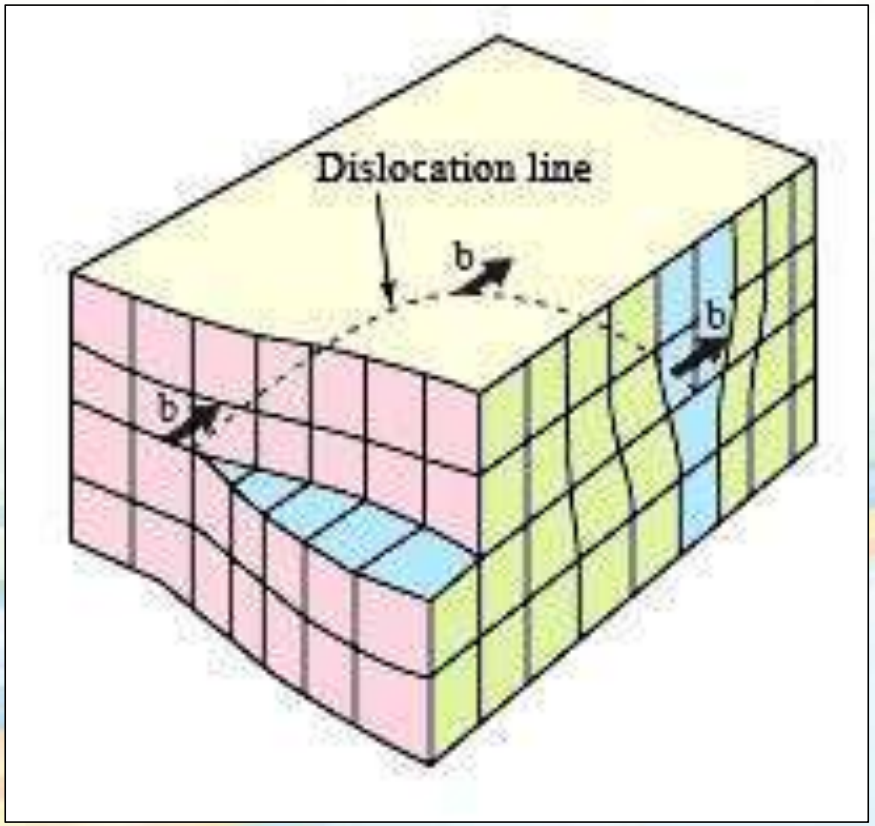
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Mixed/partial dislocations (not tested)

- The exact structure of dislocations in real crystals is usually more complicated than the ones shown in the edge and screw dislocations.
- Edge and screw dislocations are just extreme forms of the possible dislocation structures.
- Most dislocations have mixed edge/screw Character.

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Edge, Screw, and Mixed Dislocations



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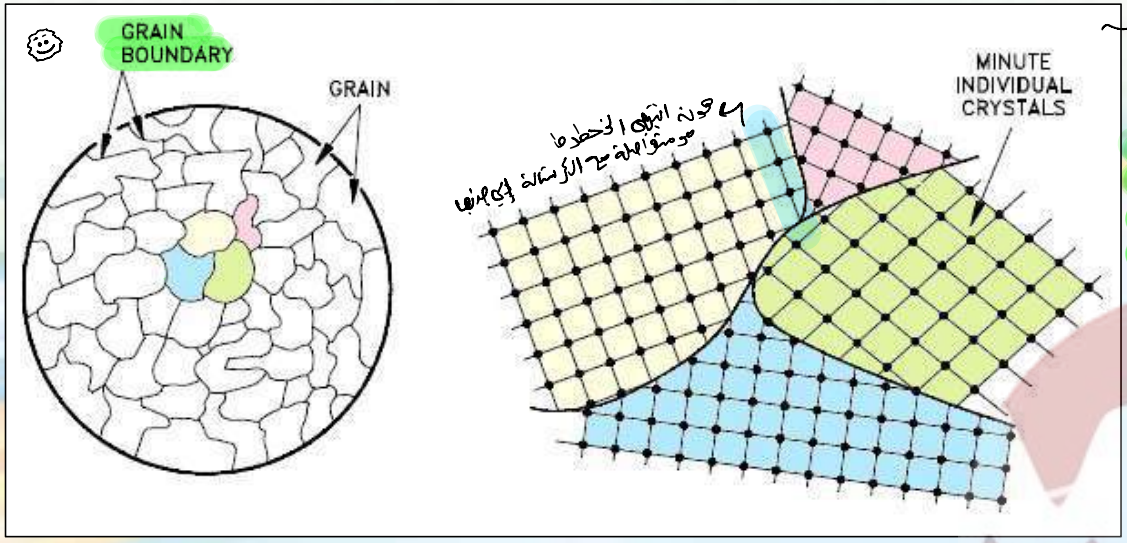
Interfacial Defects

- **Interfacial defects** are two dimensional boundaries with different crystal structures and/or orientations.
- **External surface:** where the crystal terminates.
- **Grain boundaries:** crystal often form groups of atoms known as grains, which when combined with other grains in a large crystal, often have misalignments that form boundaries.
- **Phase boundaries:** where a crystal forms more than one phase (i.e. solid and liquid)
- Polycrystalline material comprised of many small crystals or grains.
- The grains have different crystallographic orientation.

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→ As grain Boundaries Length ↑ Area defect ↑ =>

- There exist atomic mismatch within the regions where grains meet. These regions are called grain boundaries.
- Surfaces and interfaces are reactive and impurities tend to segregate there. Since energy is associated with interfaces, grains tend to grow in size at the expense of smaller grains to minimize energy.

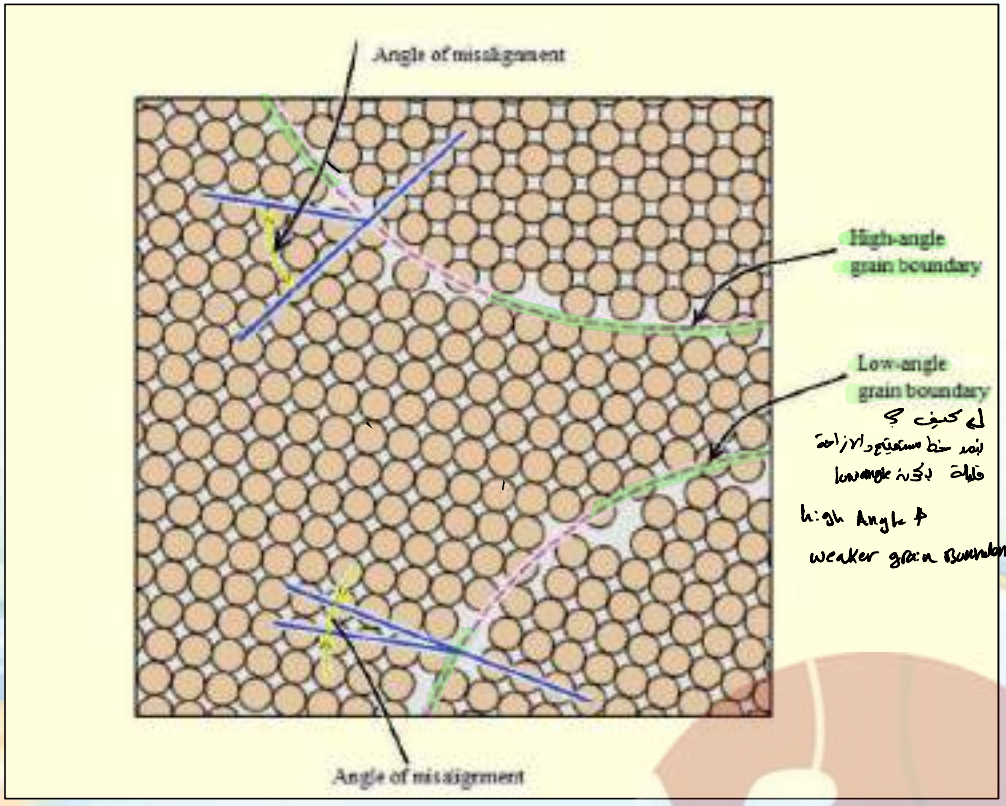


→ effects on the mechanical properties.

Factors that effect on Area defect
1) orientation
2) grain Boundary's Length

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- *High and Low Angle Grain Boundaries:*
- *Depending on misalignments of atomic planes between adjacent grains we can distinguish between the low and high angle grain boundaries*

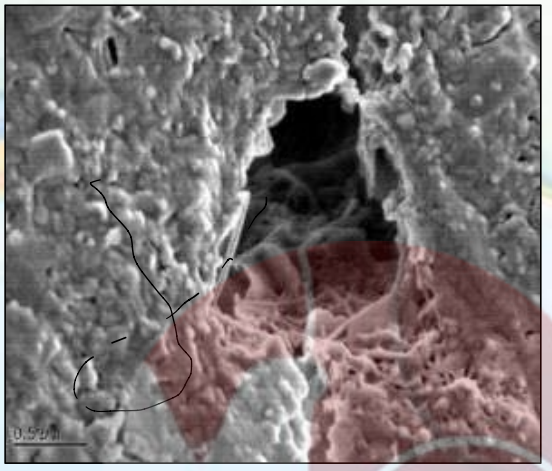


→ Most dangerous defect.

Bulk or Volume Defects

=> agglomeration of carbon in Fe it will form graphite inside steel (Fe+C) => it's a Bulk defect.

- Bulk defects occur on a much bigger scale than the rest of the crystal defects discussed.
- Voids are regions where there are a large number of atoms missing from the lattice. → cause failure of structure.
- Pores - can greatly affect optical, thermal, mechanical properties.
- Cracks - can greatly affect mechanical properties.
- Foreign inclusions - can greatly affect electrical, mechanical, optical properties
- The image is a void in a piece of metal. The image was acquired using a Scanning Electron Microscope (SEM).



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Atomic Vibrations

- Heat causes atoms to vibrate.
- Vibration amplitude increases with temperature.
- Melting occurs when vibrations are sufficient to rupture bonds.
- Vibrational frequency ~ 10^{13} Hz.
- Average atomic energy due to thermal excitation is of order kT.

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Chapter 5

Mechanical Properties

The University of Jordan
Chemical Engineering Department
First Semester 2021
Prof. Yousef Mubarak

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Outline

to know how material will behave and what's having mechanical properties by doing standard experiment work.

- **Stress and strain**

  What are they and why are they used instead of load and deformation?

- **Elastic behavior**

reversible process

⊛ deformation → change in Area (diameter) and length by increasing or reduction.

  When loads are small, how much deformation occurs? What materials deform least?

- **Plastic behavior**

irreversible process.

  At what point does permanent deformation occur? What materials are most resistant to permanent deformation?

- **Toughness and ductility**

  What are they and how do we measure them?

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Introduction

→ Stress effect on Area that will resist the Applied force

- Engineers are primarily concerned with the development and design of machines, structures etc. ⇒ Selection of Material of construction is important for design.
- These products are often subjected to forces/deformations, resulting in stresses/strains, the properties of materials under the action of forces and deformations becomes an important engineering consideration.
- The properties of materials when subjected to stresses and strains are called "mechanical properties". In other words the properties that determine the behavior of engineering mats under applied forces are called "mechanical properties".

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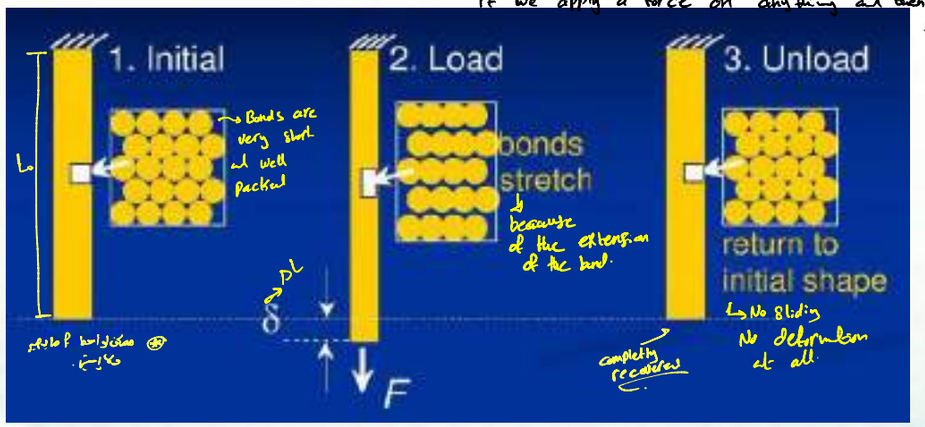
Deformation

- The response of a material to applied forces depends on the type and nature of the bond and the structural arrangement of atoms, molecules or ions.
- Basic deformation types for load carrying materials are:

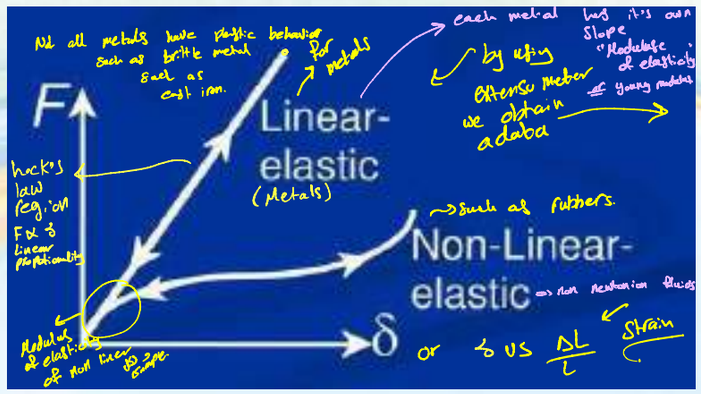
1. Elastic deformation (deformations are instantaneously recoverable)
2. Plastic deformation (non-recoverable)
3. Viscous deformation (time dependent deformation)

- There are four principal ways in which a load may be applied: namely, tension, compression, shear, and tension

Elastic Deformation

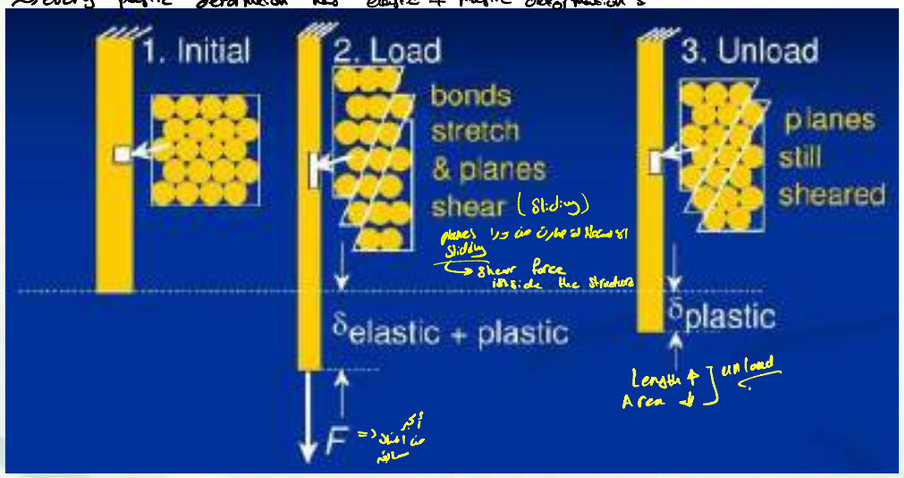


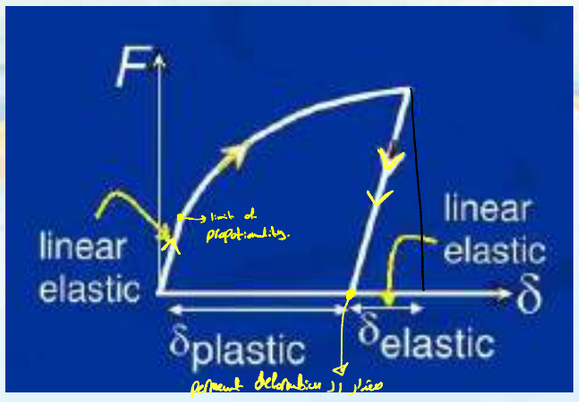
- Return to the original shape when the applied load is removed.
- Elastic means reversible!



Plastic Deformation

→ every plastic deformation has elastic + plastic deformation s





- Could not return to the original shape when the applied load is removed.
- Plastic means permanent!

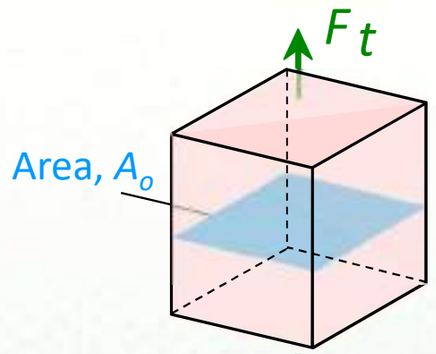
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Engineering Stress

perpindicular on the appliial resistance area. (Minimum area)

longitudinal stress.

➢ *Tensile stress* is the elongation of the material when a stretching force is applied along with the axis of applied force.



compression
tensile. use

$$\sigma = \frac{F_t}{A_0} = \frac{lb_f}{in^2} \text{ or } \frac{N}{m^2} \rightarrow Pa$$

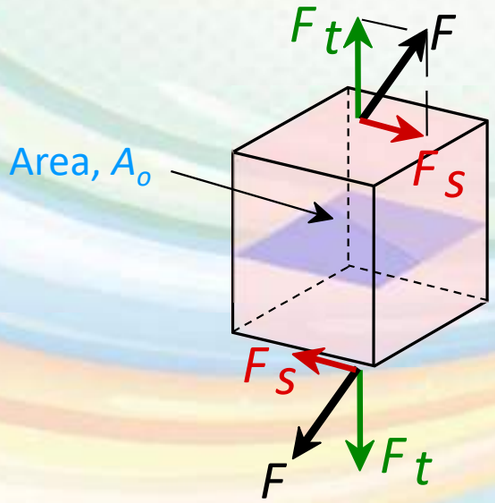
psi?

A_o is the original area before loading

Force signs:
1) +ve => tensile
2) - ve => compression

ΔL Also => +ve when
ΔL => -ve reduction of length.

inclined force => Shear + tensile.

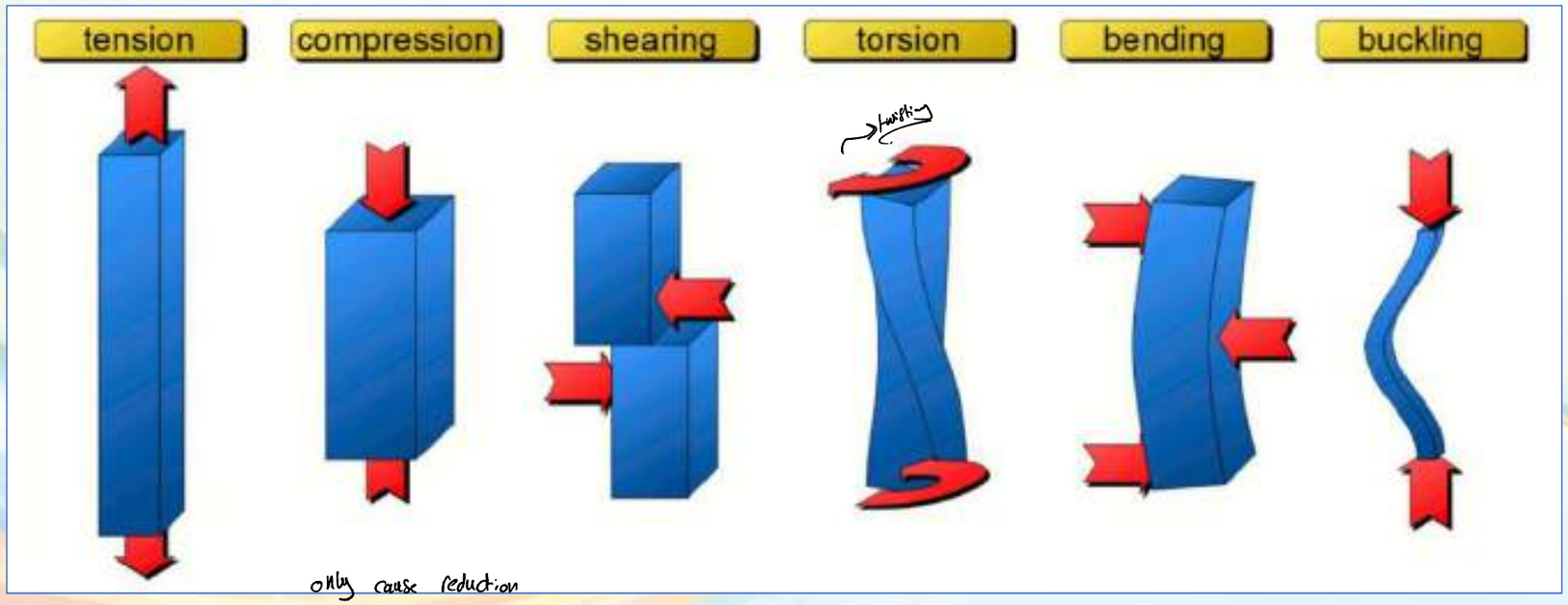


➢ *Shear stress*, is the component of stress coplanar with a material cross section. It arises from the shear force, the component of force vector parallel to the material cross section.

$$\tau = \frac{F_s}{A_0}$$

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Patterns of Deformation



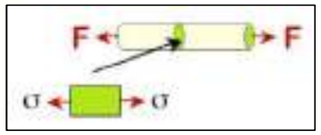
only cause reduction in length.

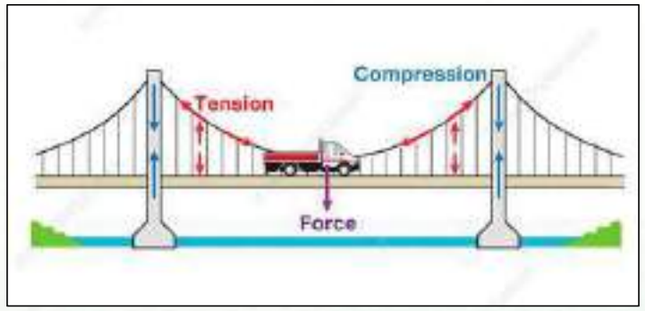
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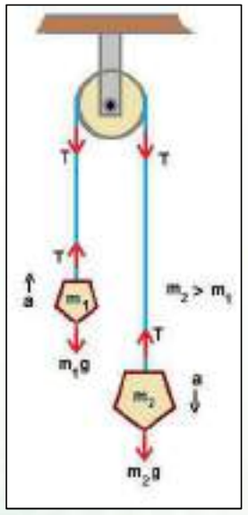
Common States of Stress

➢ **Simple tension:** $\sigma = \frac{F_t}{A_0}$



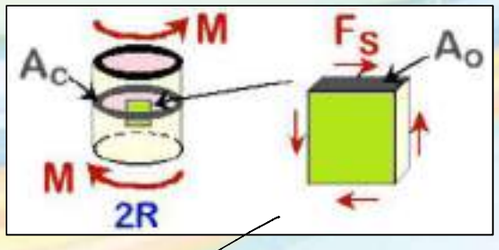


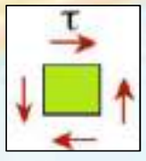




➢ **Simple shear:** $\tau = \frac{F_s}{A_0}$



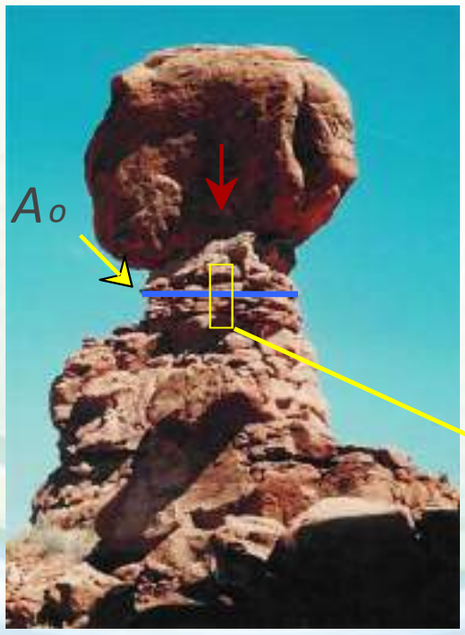




In this case, shear stress

$$\tau = \frac{M}{RA_c}$$

Simple compression:



Maximum stress @ minimum Area.



$$\sigma = \frac{F}{A_o}$$



Note: compressive structure member ($\sigma < 0$ here).

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Bi-axial tension

Pressurized tank



$\sigma_\theta > 0$

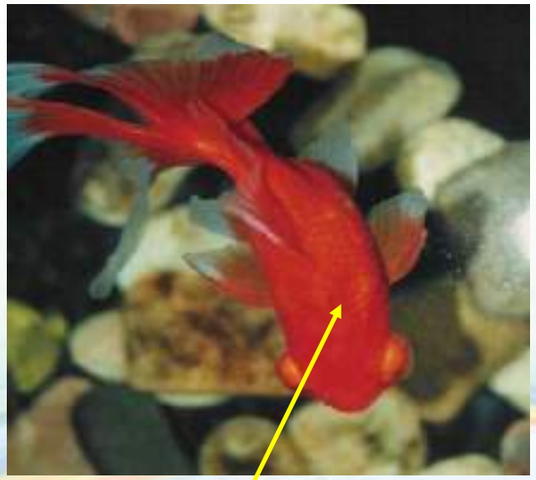
$\sigma_z > 0$

Hydrostatic compression

hydrostatic stress = pgh

higher height → higher stress.

Fish under water



$\sigma_h < 0$

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Engineering Strain

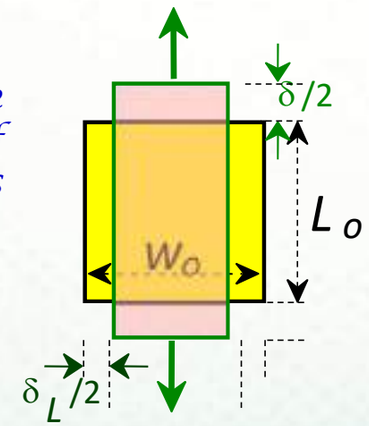
responces by the applied force

may be elastic and plastic.

Tensile strain

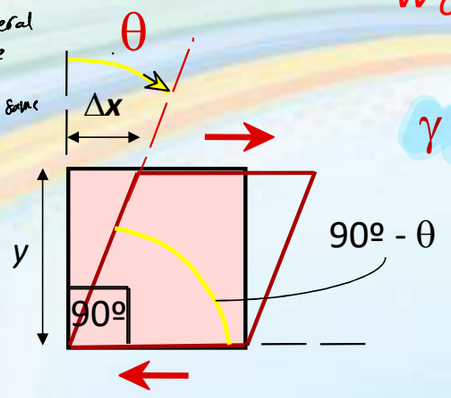
- strain is defined as the change in the shape of an object when stress is applied.
- Strain is always dimensionless.

$$\varepsilon = \frac{\delta}{L_o}$$



Shear strain

- is the ratio of the change in deformation to its original length perpendicular to the axes of the member due to shear stress. Shear stress is stress in parallel to the cross section of the structural member



$$\gamma = \Delta x / y = \tan\theta$$

poson factor = $-\left(\frac{\varepsilon_{lateral}}{\varepsilon_L}\right)$ Always +ve

0.25 ~ 0.33

Lateral strain

- Also known as transverse strain, is defined as the ratio of the change in diameter of a circular bar of a material to its diameter due to deformation in the longitudinal direction

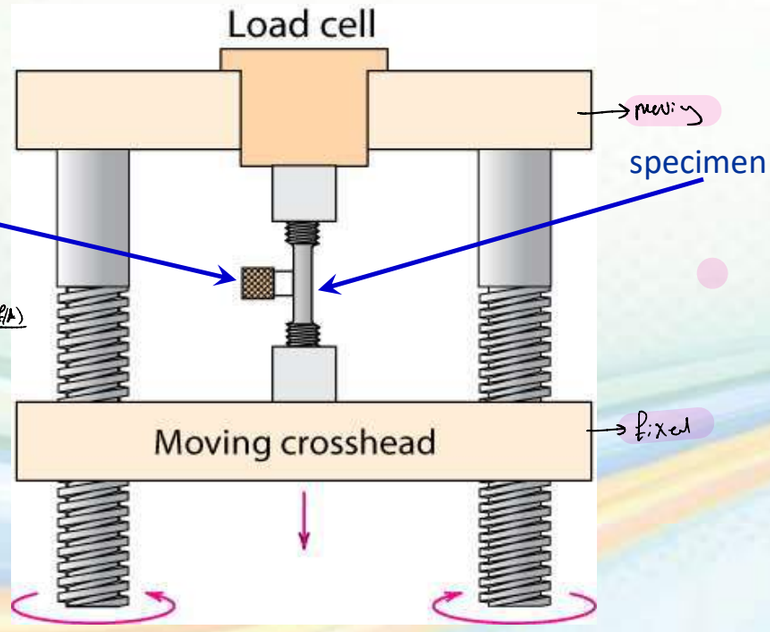
$$\varepsilon_L = \frac{-\delta_L}{W_o}$$ (reduction)

Tensile Strain ⊥ lateral Always have opposite sign but not necessary have the same value

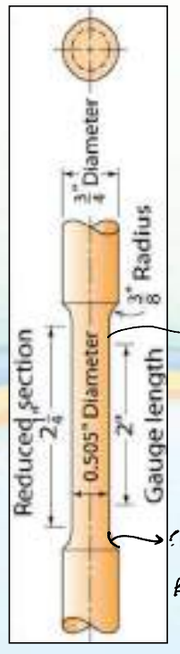
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Stress-Strain Testing

Typical tensile test machine



Typical tensile specimen



Linear Elastic Properties

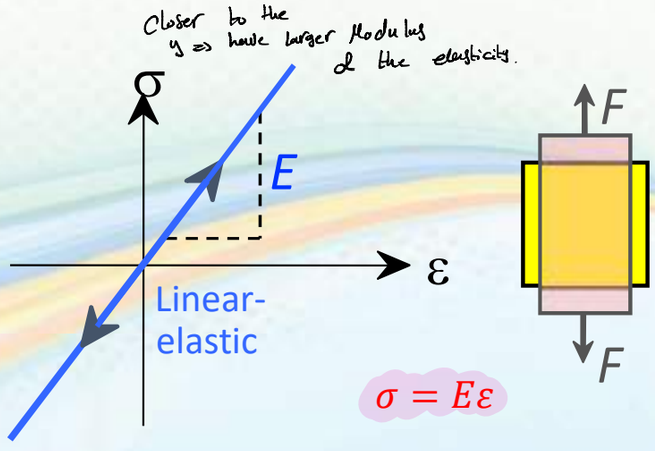
Modulus of Elasticity, E:

→ how the material will behave like elastic.

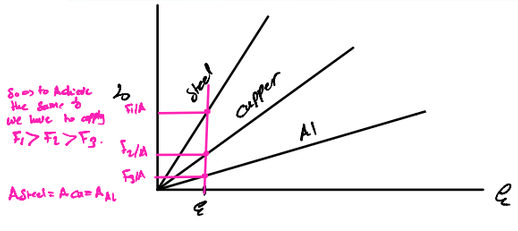
- Modulus of Elasticity, also known as Elastic Modulus or simply Modulus or Young's modulus, is the measurement of a material's elasticity. Elastic modulus quantifies a material's resistance to non-permanent, or elastic, deformation.

Hooke's Law:

- Law of elasticity discovered by the English scientist Robert Hooke in 1660, which states that, for relatively small deformations of an object, the displacement or size of the deformation is directly proportional to the deforming force or load.



Units of E: [GPa] or [psi]



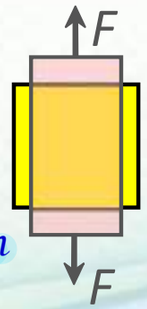
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Poisson's ratio, n

- Poisson's ratio is defined as the ratio of the change in the width per unit width of a material, to the change in its length per unit length, as a result of strain

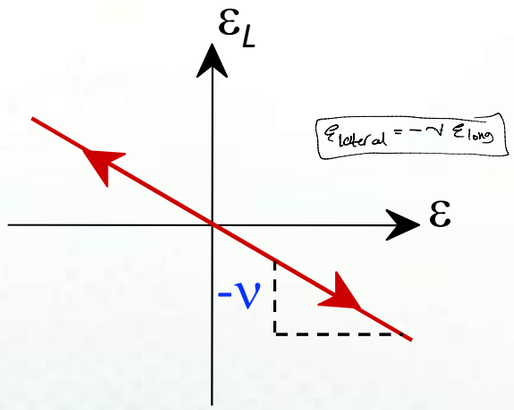
from stress–strain graph we can also determine it.

$$\nu = -\frac{\varepsilon_{Later}}{\varepsilon_{Longitudinal}}$$



- Longitudinal strain: in the direction of the applied force
- Lateral strain: in the transverse direction

- Units of ν: dimensionless

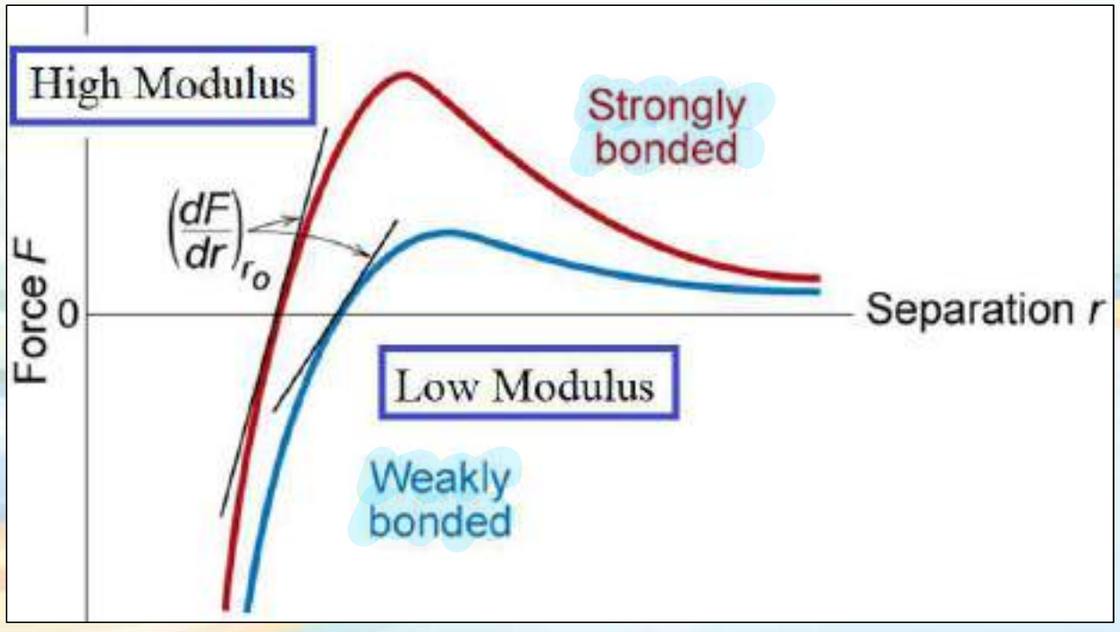


metals: ν ~ 0.33
ceramics: ν ~ 0.25
polymers: ν ~ 0.40

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Mechanical Properties

- Slope of stress strain plot (which is proportional to the elastic modulus) depends on bond strength of metal.



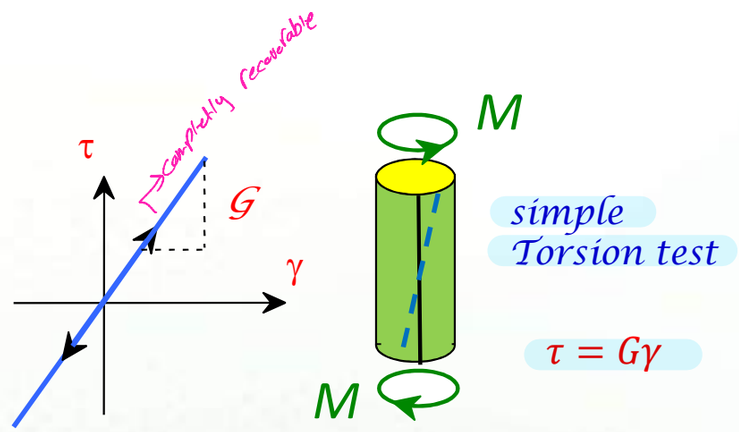
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from shear stresses.

Other Elastic Properties

Elastic Shear modulus, G: "Modulus of rigidity"

- Or the modulus of rigidity, is derived from the torsion of a cylindrical test piece. It describes the material's response to shear stress.

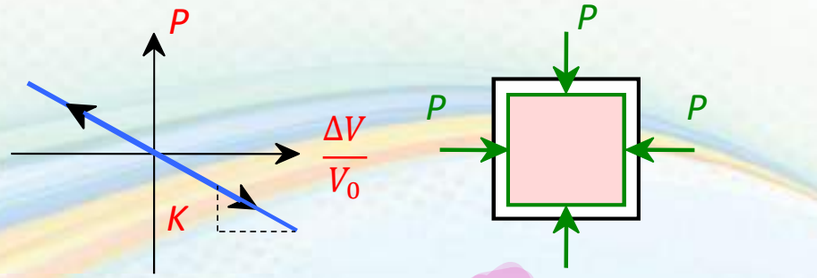


simple Torsion test

$\tau = G\gamma$

Elastic Bulk modulus, K:

- Bulk modulus, numerical constant that describes the elastic properties of a solid or fluid when it is under pressure on all surfaces. ⇒ لو التغير في Volume ولا حجم طبيعي (كوني) elastic



- Special relations for isotropic materials:

$$G = \frac{E}{2(1+\nu)}$$

$$K = \frac{E}{3(1-2\nu)}$$

$$P = -K\frac{\Delta V}{V_0}$$ → positive if we have increasing in volume (expansion)

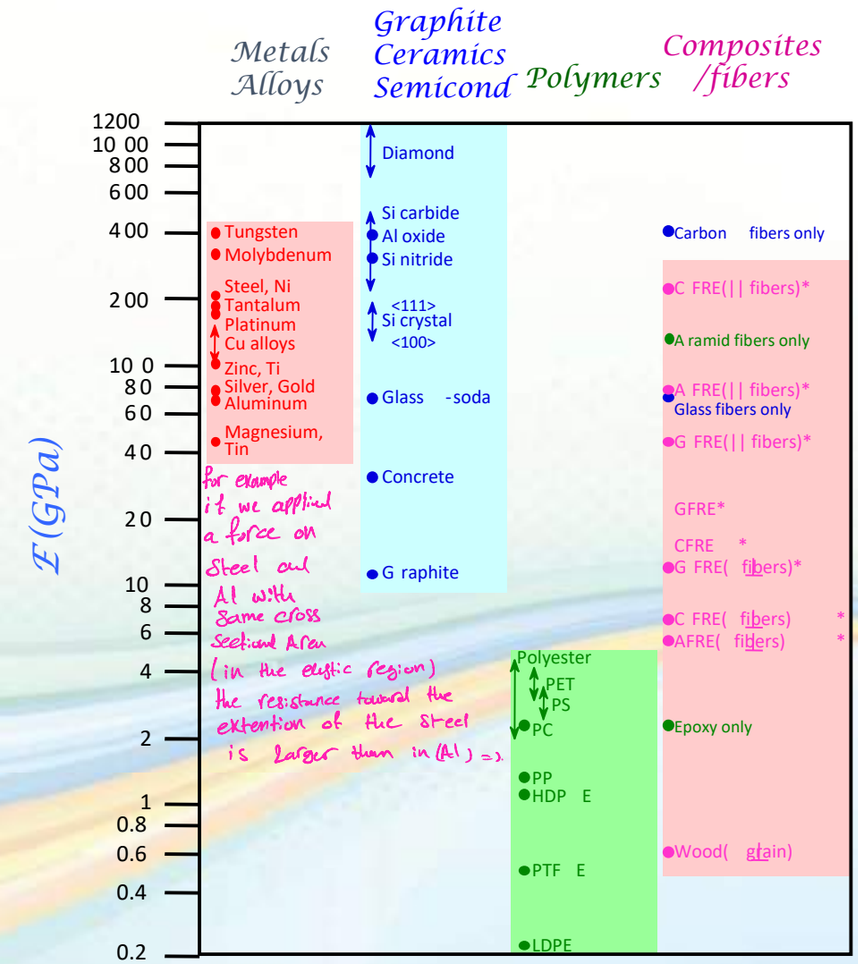
V_o = Initial volume

DV = change in volume

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Young's Moduli: Comparison

Gpa = 10^9 Pa



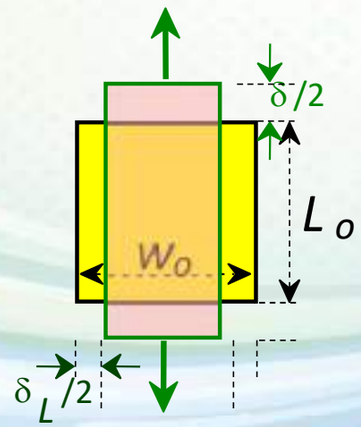
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Useful Linear Elastic Relationships

Simple tension

$$\delta = \frac{F L_0}{E A_0}$$

$$\delta_L = -\nu \frac{F w_0}{E A_0}$$

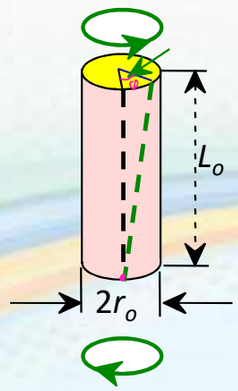


Simple torsion

$$\alpha = \frac{2 M L_0}{\pi r_0^4 G}$$

$\mathcal{M}$ = moment

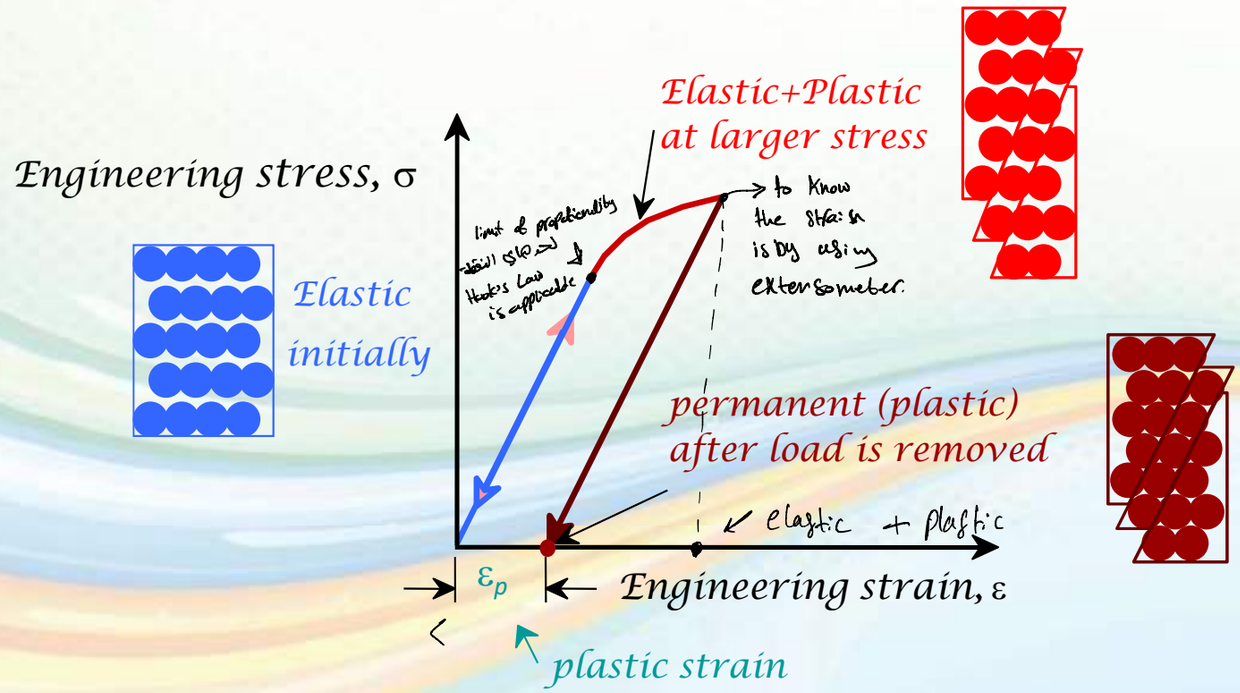
α = angle of twist



- Material, geometric, and loading parameters all contribute to deflection.
- Larger elastic moduli minimize elastic deflection.

Plastic (Permanent) Deformation

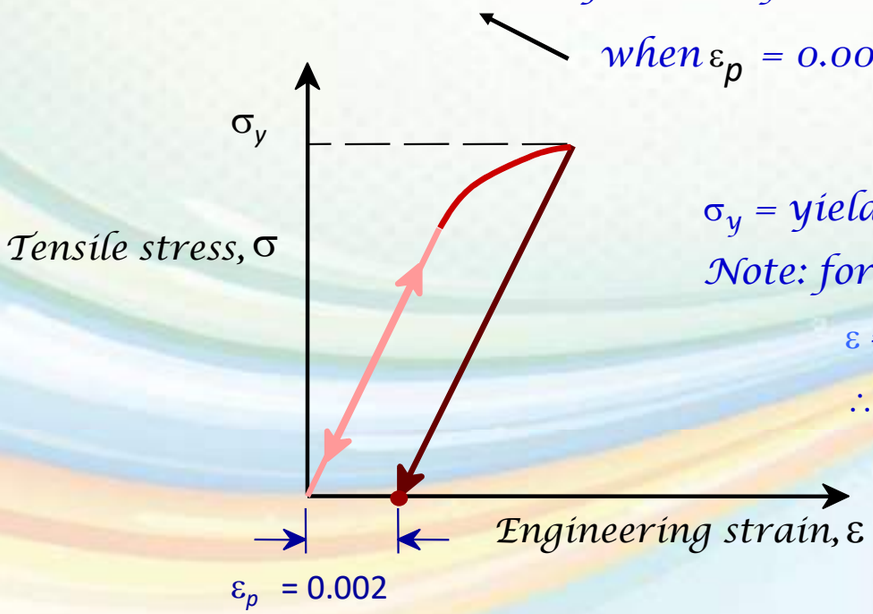
➢ **Simple tension test** (at lower temperatures, i.e. $T < T_{melt/3}$)



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Yield Strength, σ_y

- The yield strength is defined as the stress at which a predetermined amount of permanent deformation occurs. The graphical portion of the early stages of a tension test is used to evaluate yield strength.
- Stress at which **noticeable** plastic deformation has occurred.



σ_y = yield strength

Note: for 2 inch sample

$\varepsilon = 0.002 = \Delta z / z$

$\therefore \Delta z = 0.004$ in

G yield at a "value" of strain ⇒ No yield region

↳ yield stress = value There is a yield region

⊛ لما عندي منطقة yield وأنا صايدي أتجاوز قيمة strain معينة

يعني أحدد الـ force ماكسيموم بحيث عن طريقه إني أحدده

من الرحمة إني أحدد حتى موازي لحد ما أحتاجها بالرحمة

حتى المنطقة رح أقرأ منها قيمة الـ stress بعد ما يصير

$F = A \cdot \sigma$ ⇒ هيك بقدر

أعرف ده.

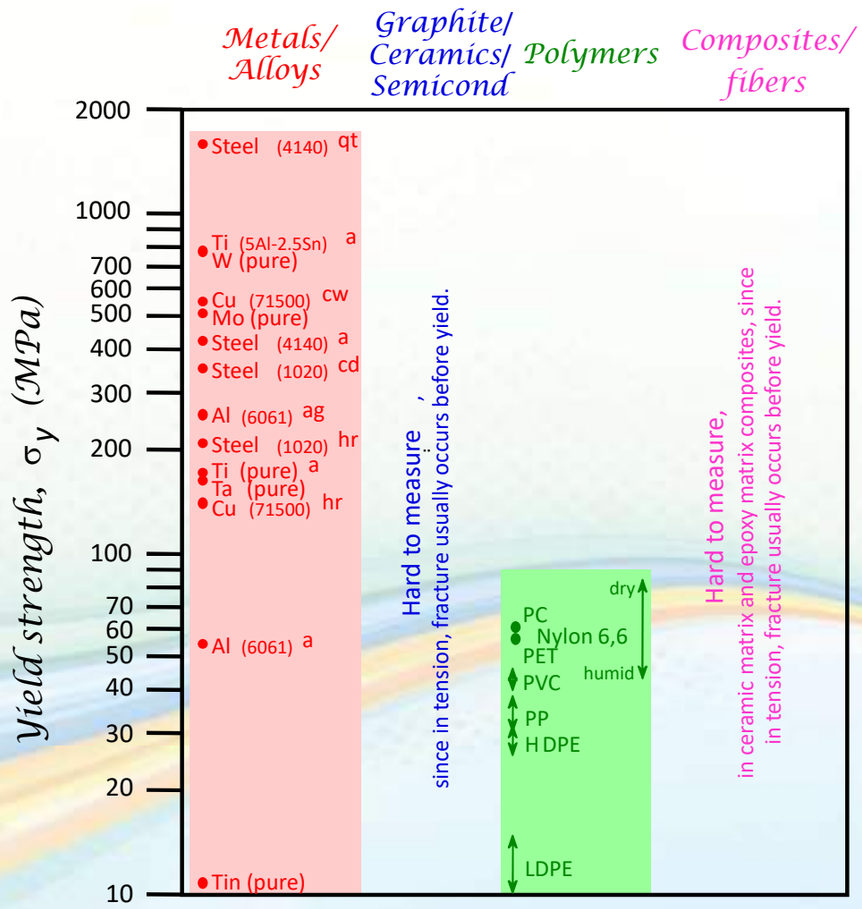
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Yield Strength: Comparison

Room temperature values

Based on data in Table B.4, Callister & Rethwisch 8e.

a = annealed
hr = hot rolled
ag = aged
cd = cold drawn
cw = cold worked
qt = quenched & tempered



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Tensile Strength, TS

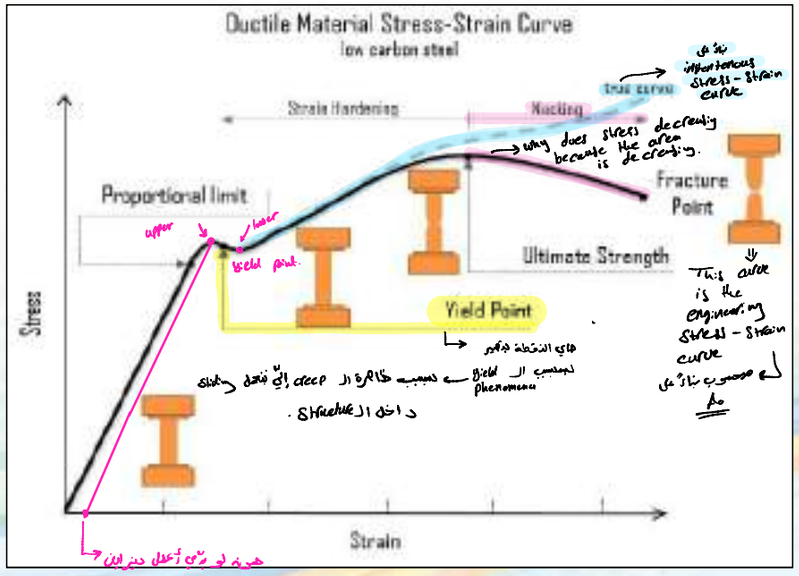
- Maximum stress on engineering stress-strain curve.

Design stress = Maximum stress

working stress = Max. stress / factor of safety

as it larger than ① it is better and safer

* if we choose yield region technically it is in the elastic especially if we consider it as working stress.



- Metals: occurs when noticeable necking starts.
- Polymers: occurs when polymer backbone chains are aligned and about to break.

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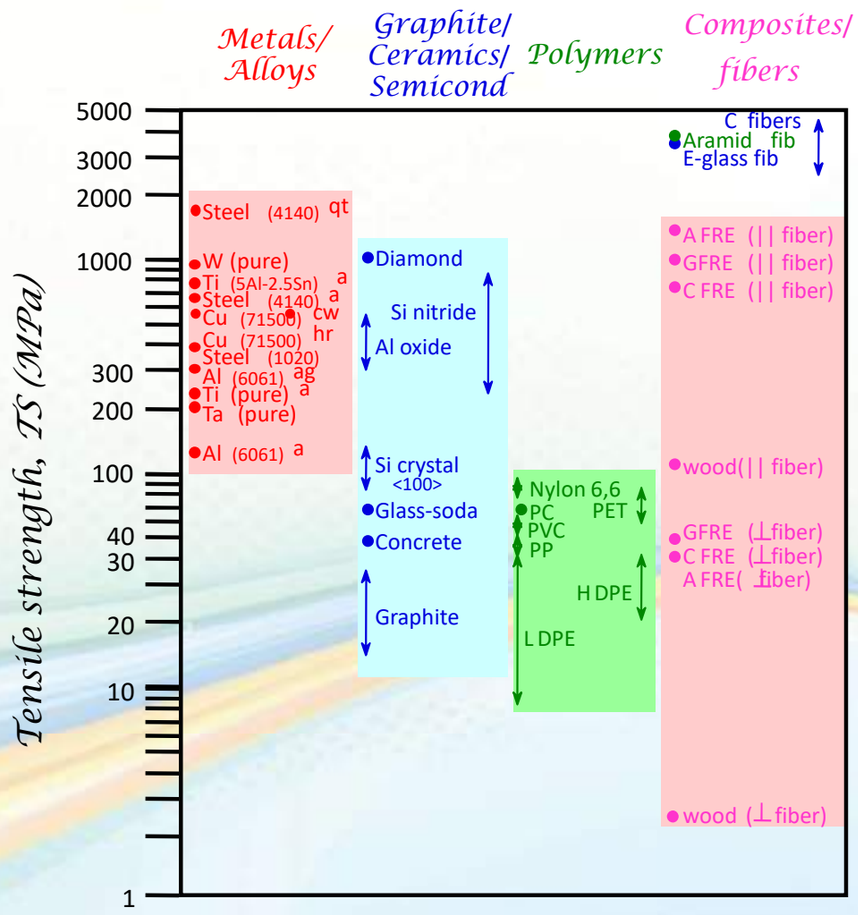
Tensile Strength: Comparison

Room temperature values

Based on data in Table B.4, Callister & Rethwisch 8e.

a = annealed
hr = hot rolled
ag = aged
cd = cold drawn
cw = cold worked
qt = quenched & tempered

AFRE, GFRE, & CFRE = aramid, glass, & carbon fiber-reinforced epoxy composites, with 60 vol% fibers.



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خاصية لكل سنحتاج . قبل ما أكمل

Ductility

- Ductility is the physical property of a material associated with the ability to be hammered thin or stretched into wire without breaking. A ductile substance can be drawn into a wire.

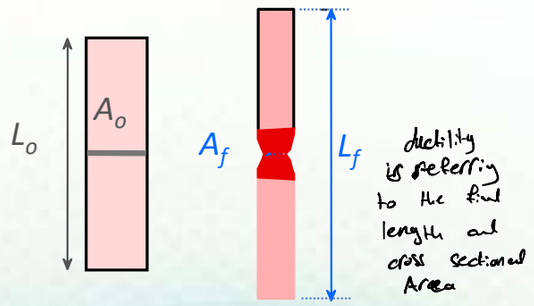
- Plastic tensile strain at failure:

$$\%EL = \frac{L_f - L_o}{L_o} \times 100$$

Variation ↑ ductile ↑

for compression $L_o > L_f$

$\frac{L_o - L_f}{L_o}$ ×100%

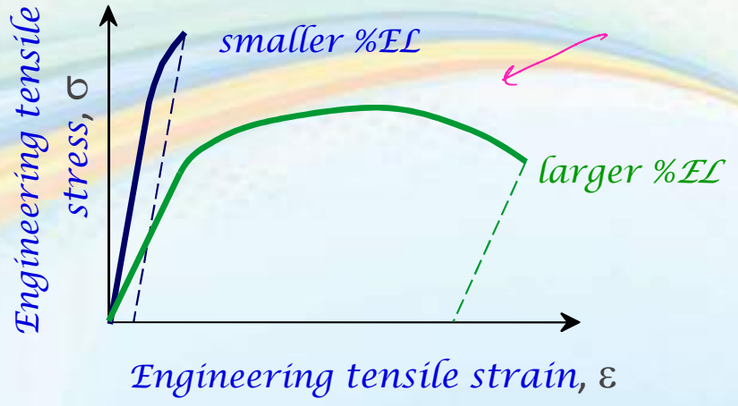


- Another ductility measure:

$$\%RA = \frac{A_o - A_f}{A_o} \times 100$$

Cant for brittle material

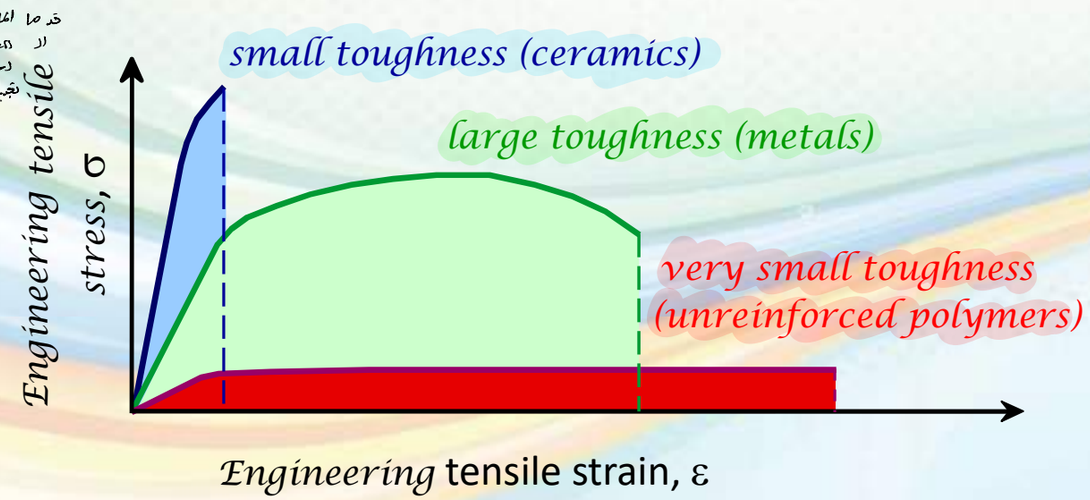
ductility approaches to zero because $|L_o - L_f| \approx$ zero.



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Toughness

- Toughness is a fundamental material property measuring the ability of a material to absorb energy and withstand shock up to fracture; that is, the ability to absorb energy in the plastic range.
- Energy to break a unit volume of material
- Approximate by the area under the stress-strain curve.



Brittle fracture: → mainly elastic and a little plastic

elastic energy

Ductile fracture:

elastic + plastic energy

Resilience, Ur

- The ability of a material to absorb energy when deformed elastically and to return it when unloaded is called resilience.
- Ability of a material to store energy .
- Energy stored best in elastic region

$$U_r = \int_0^{\varepsilon_y} \sigma d\varepsilon$$

- If we assume a linear stress-strain curve this simplifies to:

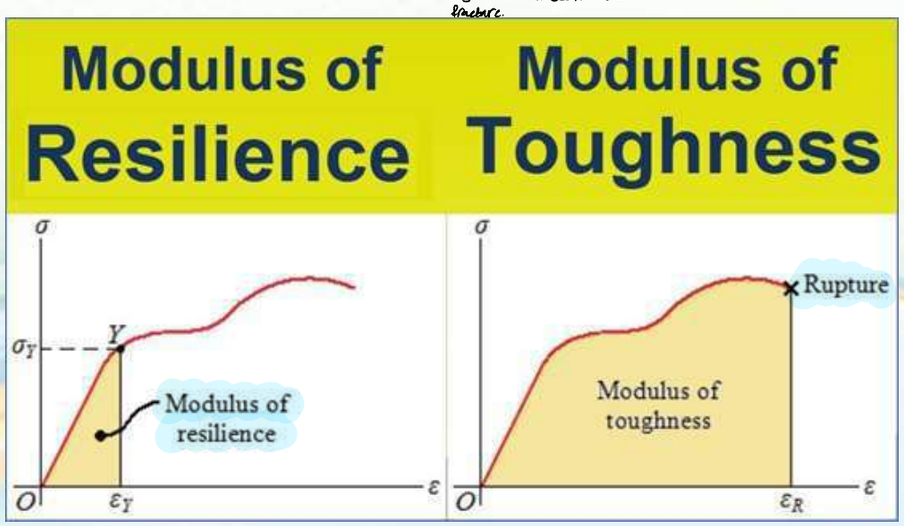
$$U_r \cong \frac{1}{2}\sigma_y \varepsilon_y$$

→ toughness ⇒ energy absorbed until fracture point (elastic + plastic)

sub Resilience ⇒ energy absorbed in the elastic region

sub necessary that will occure the fracture.

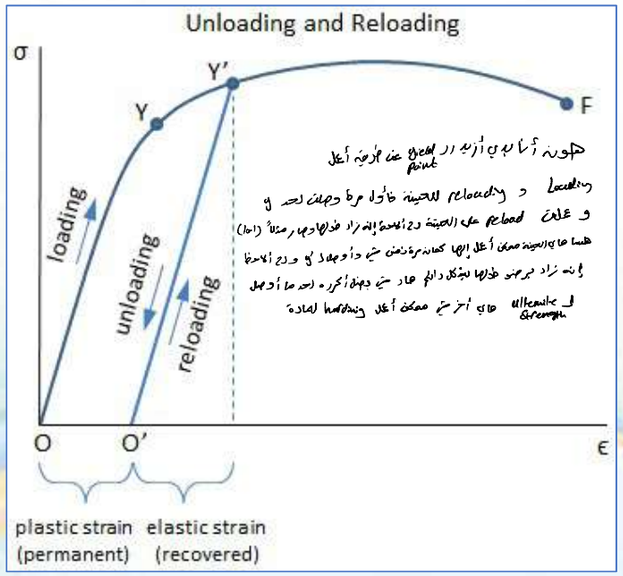
ductile material has toughness > br: He but resilience we cannot compare while we calculate the area. ⎫ Modulus of elasticity & Resilience ↓



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Elastic Strain Recovery (hardening process)

- If a material is loaded beyond the elastic limit, it will undergo permanent deformation. After unloading the material, the elastic strain will be recovered (return to zero) but the plastic strain will remain.
- The figure shows the stress-strain curve of a material that was loaded beyond the yield point, Y.
- The first time the material was loaded, the stress and strain followed the curve O-Y-Y', and then the load was removed once the stress reached the point Y'.



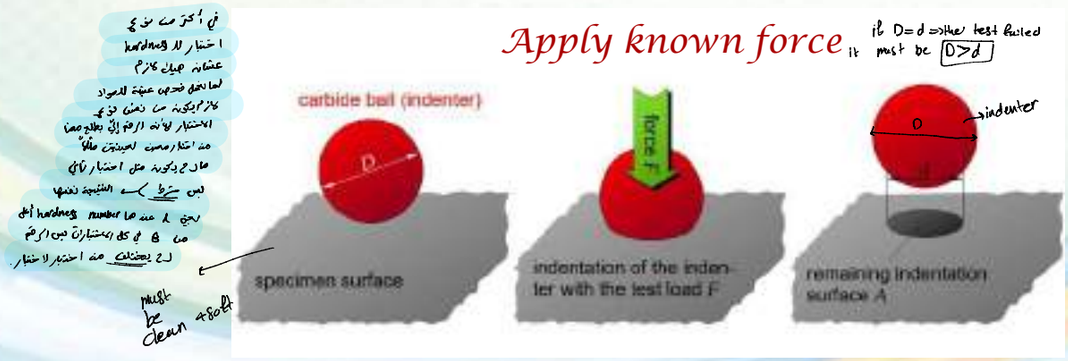
Elastic Strain Recovery

- Since the material was loaded beyond the elastic limit, only the elastic portion of the strain is recovered, there is some permanent strain now in the material.
- If the material were to be loaded again, it would follow line O'-Y'-F, where O'-Y' is the previous unloading line.
- The point Y' is the new yield point. Note that the line O'-Y' is linear with a slope equal to the elastic modulus, and the point Y' has a higher stress value than point Y.
- Therefore, the material now has a higher yield point than it had previously, which is a result of strain hardening that occurred by loading the material beyond the elastic limit.

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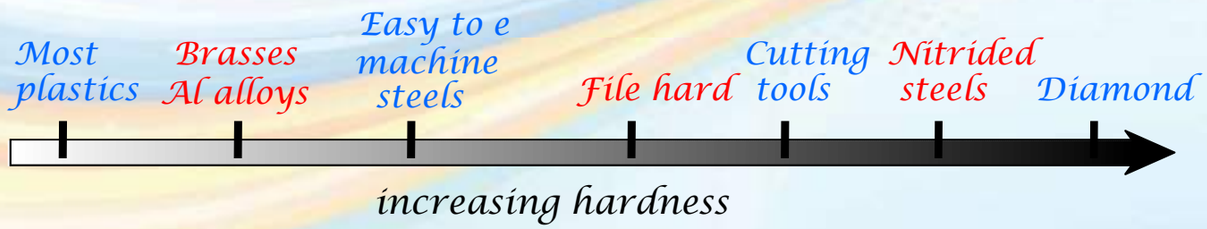
Hardness

- Resistance to permanently indenting the surface.
- Large hardness means:
  - ✓ Resistance to plastic deformation or cracking in compression.
  - ✓ Better wear properties.



Measure size of indent after removing load

Smaller indents mean larger hardness.



Hardness: Measurement

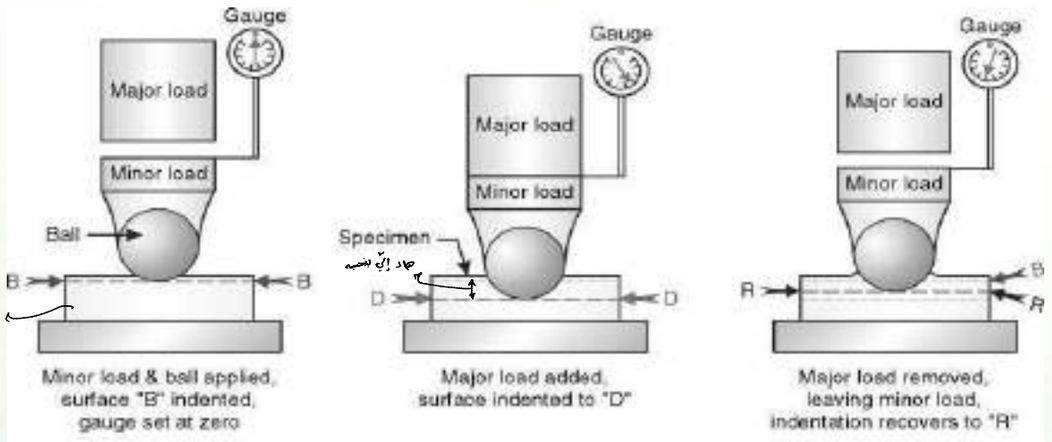
Rockwell

The Rockwell method measures the permanent depth of indentation produced by a force/load on an indenter.

↳ two loads ← minor load, major load

- No major sample damage
- Each scale runs to 130 but only useful in range 20-100.
- Minor load 10 kg
- Major load 60 (A), 100 (B) & 150 (C) kg
  - A = diamond, B = 1/16 in. ball, C = diamond

- HB = Brinell Hardness
  - TS (psia) = 500 x HB
  - TS (MPa) = 3.45 x HB

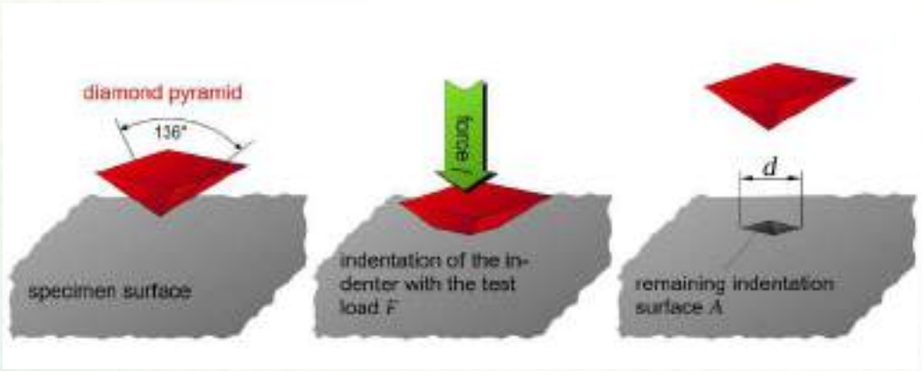


Distance RB is used to calculate Rockwell hardness, or read directly from the gauge

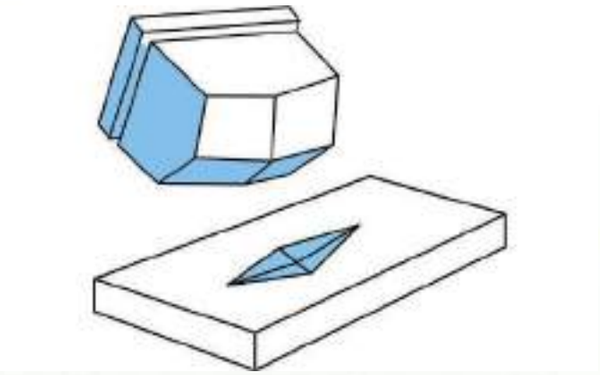


Rockwell Hardness Apparatus

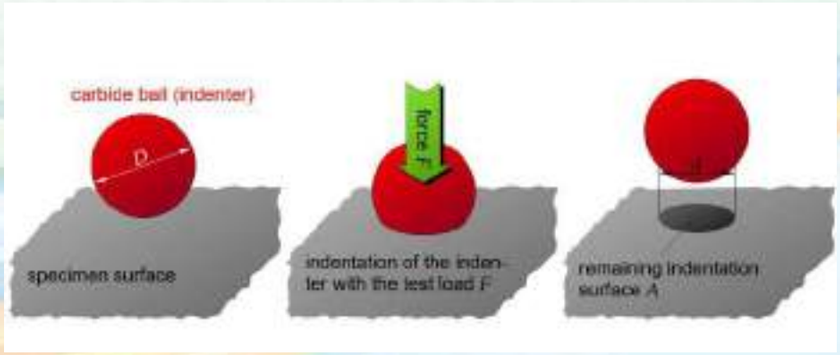
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Vickers



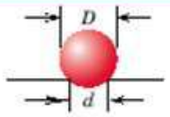
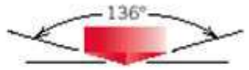
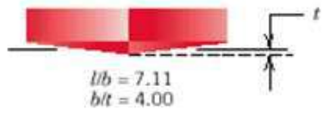
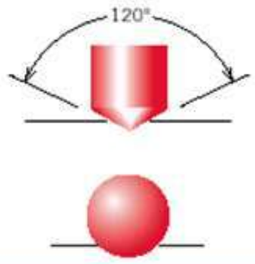
Knoop



Brinell

Hardness: Measurement

Table 6.4 Hardness Testing Techniques

Test	Indenter	Shape of Indentation: Side View	Shape of Indentation: Top View	Load	Formula for Hardness Number[a]
Brinell	10-mm sphere of steel or tungsten carbide			P	$\mathrm{HB} = \dfrac{2P}{\pi D[D - \sqrt{D^2 - d^2}]}$
Vickers microhardness	Diamond pyramid			P	$\mathrm{HV} = 1.854P/d_1^2$
Knoop microhardness	Diamond pyramid			P	$\mathrm{HK} = 14.2P/l^2$
Rockwell and Superficial Rockwell	Diamond cone $\frac{1}{16}, \frac{1}{8}, \frac{1}{4}, \frac{1}{2}$ in. diameter steel spheres			60 kg, 100 kg, 150 kg: Rockwell 15 kg, 30 kg, 45 kg: Superficial Rockwell	

[a] For the hardness formulas given, P (the applied load) is in kg, while D, d, d_1, and l are all in mm.

Chapter 6
Mechanical Failure

The University of Jordan
Chemical Engineering Department
First Semester 2021
Prof. Yousef Mubarak

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Outline

- How do Materials Break?
  - Ductile vs. brittle fracture ⇒ Based on surface of the material
- Principles of fracture mechanics
  - Stress concentration
- Impact fracture testing ⇒ response of the material because of a sudden force
- Fatigue (cyclic stresses)
  - Cyclic stresses, the S—N curve
  - Crack initiation and propagation
  - Factors that affect fatigue behavior
- Creep (time dependent deformation)
  - Stress and temperature effects
  - Alloys for high-temperature use

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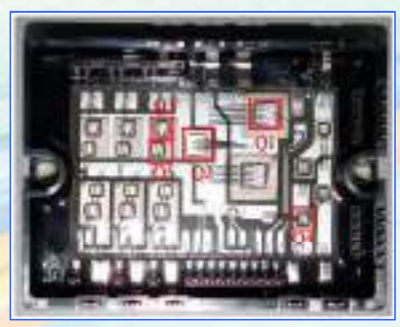
ISSUES TO ADDRESS...

- How do cracks that lead to failure form?
- How is fracture resistance quantified? How do the fracture resistances of the different material classes compare?
- How do we estimate the stress to fracture?
- How do loading rate, loading history, and temperature affect the failure behavior of materials?



Ship-cyclic loading from waves

→ fatigue



Computer chip-cyclic thermal loading

→ fatigue



Hip implant-cyclic loading from walking

→ fatigue

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Why study failure?

- Design of a component or structure: Minimize failure possibility => May lead to a disaster.
- It can be accomplished by understanding the mechanics of failure modes and applying appropriate design principles.
- Failure cost
  1. Human life
  2. Economic loss
  3. Unavailability of service
- Failure causes
  1. Improper material selection
  2. Inadequate design => thickness, shape
  3. Processing => operating conditions (T, P, —)
- Regular inspection, repair and replacement critical to safe design.
  ↳ we have to do it
  Even if we select good material of construction, processing, etc.

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Fracture => one type of failure.

- Fracture is the separation of a body into (at least) two or more pieces in response to an imposed stress.

  Separation of two or more pieces
  ↳ depends on the nature of the material.

- Steps in fracture:

  1. Crack formation ← small voidage because of defects ← impurities, second phase, etc.
  2. Crack propagation → slow => ductile
     → fast => brittle.

⊛ Crack Always takes places in the plastic region

- Depending on the ability of material to undergo plastic deformation before the fracture two modes can be defined:

  1. Ductile fracture (elongation ↑, reduction in cross sectional Area)
     ↳ the material is more ductile
     the fracture will occure in the minimum cross Sectional Area
  2. Brittle fracture

⊛ Some of ductile materials can be a brittle (even if its very ductile)
↳ by cooling to a certain temperature (as long as the temperature is like that => the material will remain brittle.)

⊛ أمثلة على مواد Brittle و ductile
عندما تتكسر كلما كانت أطول ومساحتها أقل
ductile (بالمقارنة مع الأخرى) لها تكون
Brittle عكس لوحة الرخام التي تكسر لأسفل طول ولا مساحة قوية

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Fracture Modes

Ductile fracture

- Most metals (not too cold) exhibit ductile fracture.
- Extensive plastic deformation ahead of crack.
- Crack is "stable": resists further extension unless applied stress in increased.

Brittle fracture

- Ceramics, ice, cold metals exhibit brittle fracture.
- Relatively little plastic deformation
- Crack is "unstable": propagates rapidly without increase in applied stress.
- Catastrophic

- Ductile fracture is preferred in most applications.

Ductile vs Brittle Failure

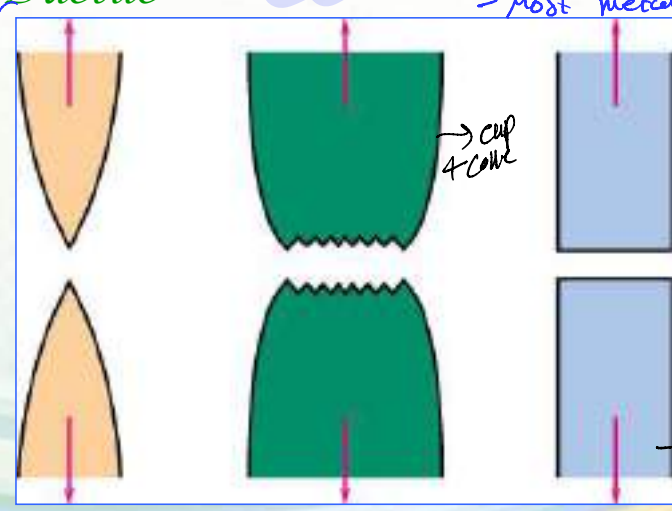
Based on the final shape after the fracture

- Classification:

Fracture behavior: Very Ductile | Moderately Ductile → Most metals | Brittle

topography of the surface is smooth + no variation in cross sectional Area (or not noticible)

Crack in Brittle material is unstable



%AR or %EL: Large | Moderate | Small

- *Very ductile*, soft metals (Pb, Au) at room temperature, other metals, polymers, glasses at high temperature.
- *Moderately ductile* fracture, typical for ductile metals.
- *Brittle fracture*, cold metals, ceramics

Ductile fracture is usually more desirable than brittle fracture!	Ductile: Warning before fracture	Brittle: No warning

elastic deformation (deviation) plastic

elongation / reduction in cross-section Area

* ductile there is a warning before the fracture unlike the brittle.

Yousef Mubarak Materials Science

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Example: Pipe Failures

- **Ductile failure:**
  - One piece
  - Large deformation

التغير الطول + مساحة



- **Brittle failure:**
  - Many pieces
  - Small deformations

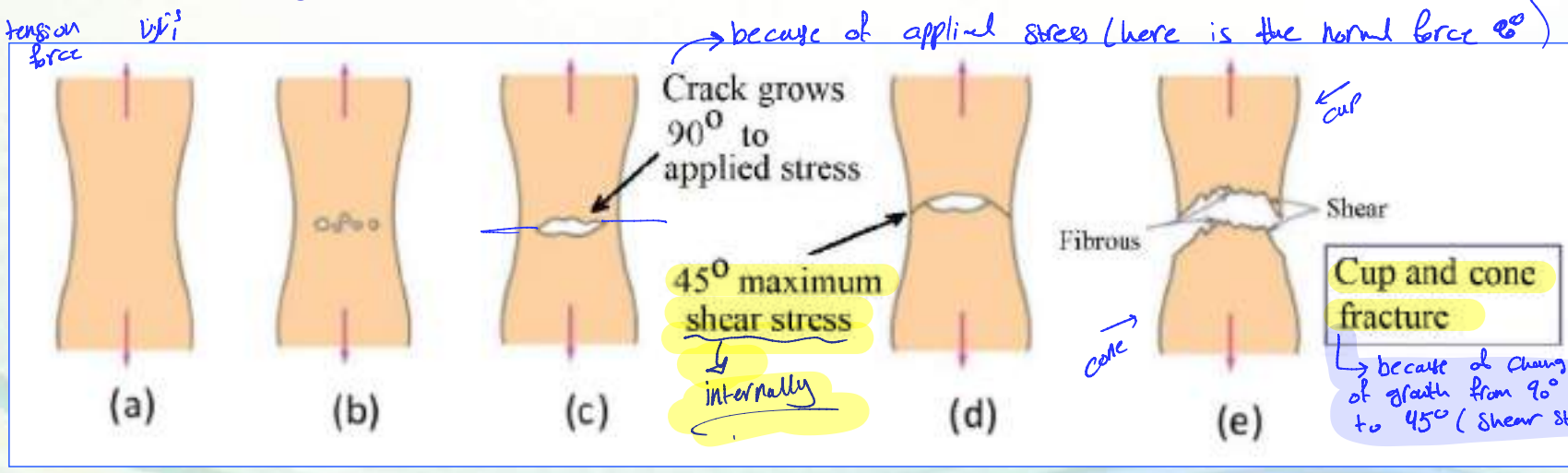
وصلى صغيرة !!



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Ductile fracture → Large reduction in cross section Area
Large extention in length
cup and cone structure.

Failure stages:



(a) Necking
(b) Formation of microvoids (micro cracks)
(c) Coalescence of microvoids to form a crack =>
(d) Crack propagation by shear deformation
(e) Fracture

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Moderately Ductile vs. Brittle Failure



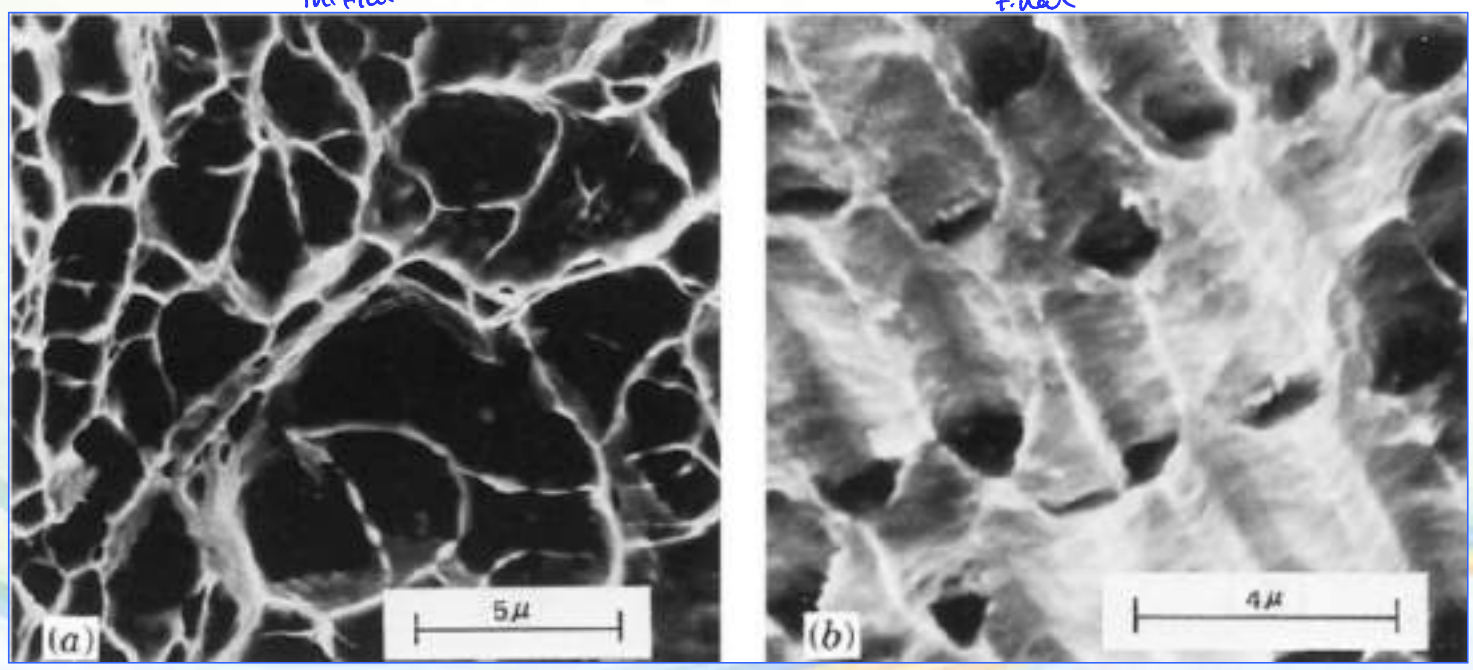
Cup-and-cone fracture in ductile Al



Brittle fracture in mild steel

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Ductile fracture



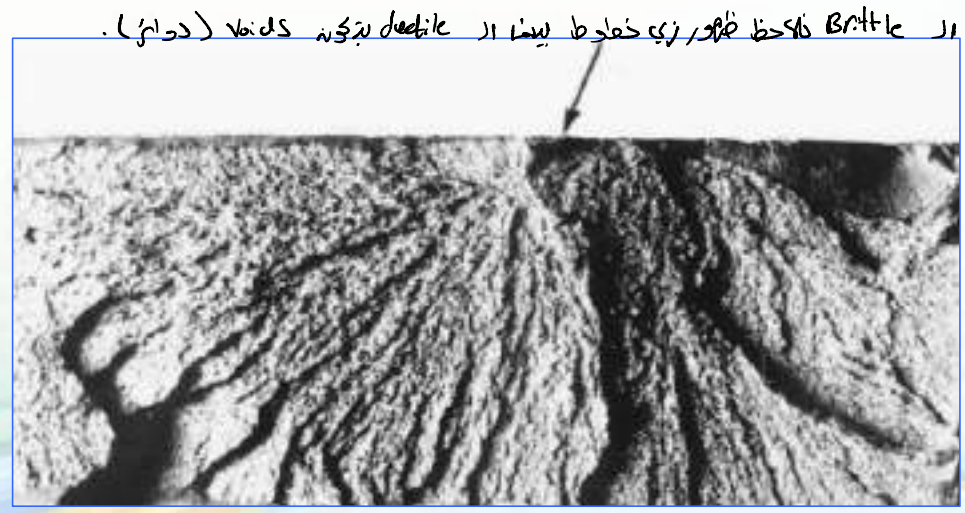
(a) SEM image showing spherical dimples resulting from a uniaxial tensile load representing microvoids. (b) SEM image of parabolic dimples from shear loading.

Brittle Failure



Red circles with arrows indicate point at which failure originated

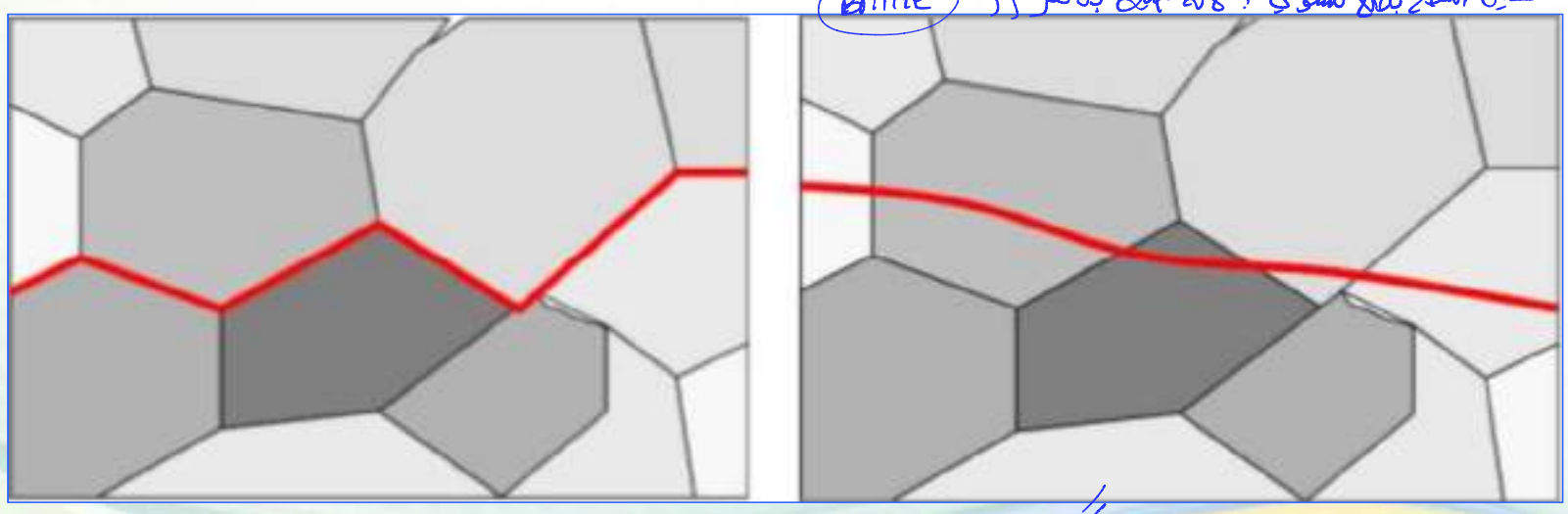
الـ Brittle نلاحظ ظهور خطوط بيضا الـ dimple بتكون voids (دوائر).



Lines or ridges that radiate from the origin of the crack in a fanlike pattern

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Brittle Fracture Surfaces



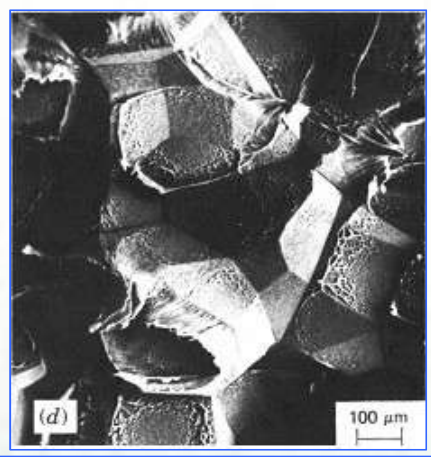
Intergranular fracture:
Fracture crack propagation is along grain boundaries (grain boundaries are weakened or embrittled by impurities segregation etc.)

Transgranular fracture:
Fracture cracks pass through grains. Fracture surface faceted texture because of different orientation of cleavage planes in grains.

Brittle Fracture Surfaces

Intergranular (between grains)

304 S. Steel (metal)

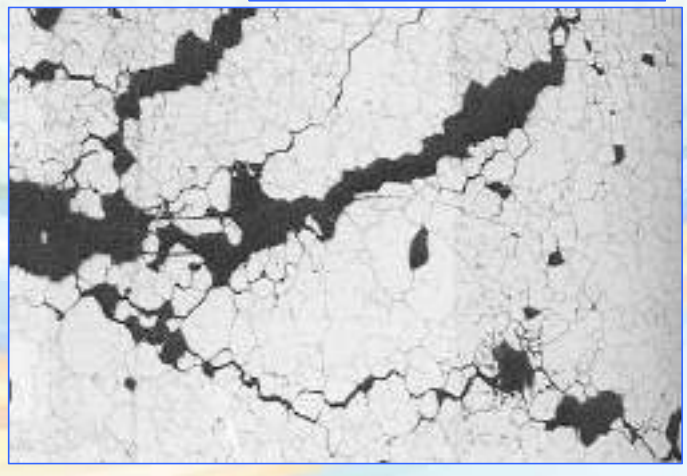




Transgranular (through grains)

S. Steel (metal)

Polypropylene (polymer)





Al Oxide (ceramic)

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Brittle Fracture (Limited Dislocation Mobility)

- No appreciable plastic deformation.
- Crack propagation is very fast
- Crack propagates nearly perpendicular to the direction of the applied stress. ⇒ 90° عمودي
  45° , لو 90° لا ← ductile
- Crack often propagates by cleavage- breaking of atomic bonds along specific crystallographic planes (cleavage planes).



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Fracture Mechanics

Studies the relationships between:

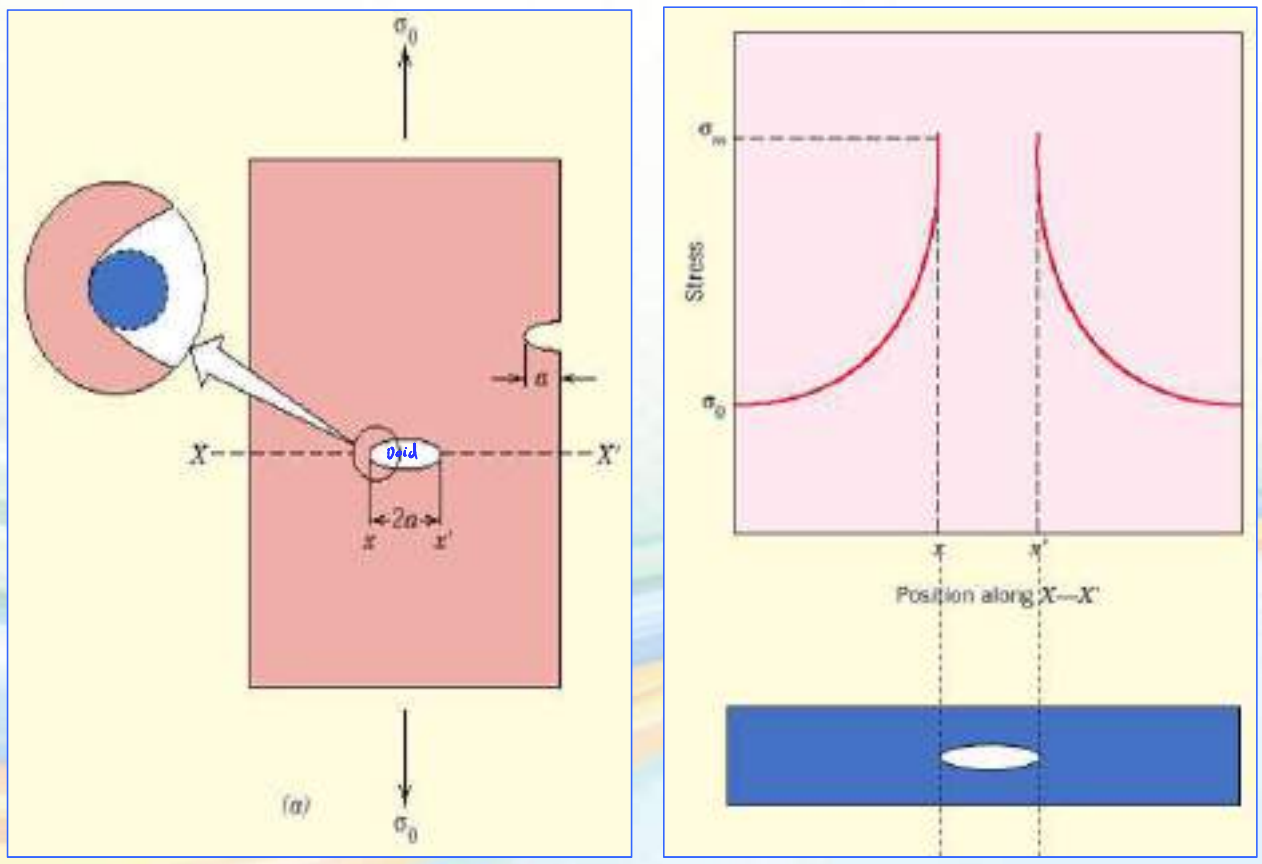
1. Material properties
2. Stress level
3. Crack producing flaws
4. Crack propagation mechanisms

Stress Concentration

- Measured fracture strength is much lower than predicted by calculations based on atomic bond energies. This discrepancy is explained by the presence of flaws or cracks in the materials.
- The flaws act as stress concentrators or stress raisers, amplifying the stress at a given point.
- The magnitude of amplification depends on crack geometry and orientation

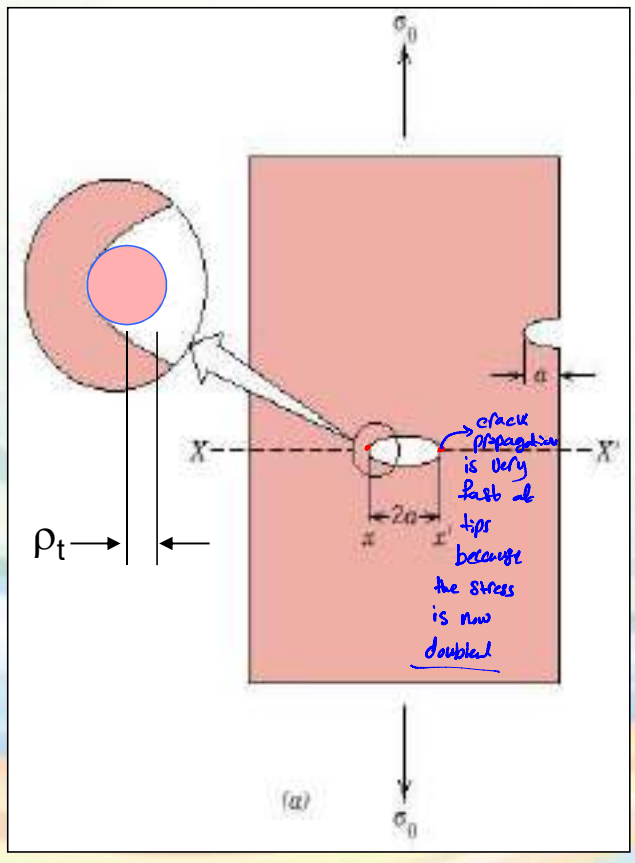
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Concentration of Stress at Crack Tip



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Flaws are Stress Concentrators



- *If the crack is similar to an elliptical hole through plate, and is oriented perpendicular to applied stress, the maximum stress, at crack tip*

$$\sigma_m = 2\sigma_o \left(\frac{a}{\rho_t}\right)^{1/2} = K_t \sigma_o$$

circle ⇐ $a = \rho_t$ and not ellipse.

where

ρ_t = *radius of curvature*

σ_o = *applied stress*

σ_m = *stress at crack tip*

a = length of surface crack or ½ length of internal crack → it's equal to a if it's on the surface

K_t = *stress concentration factor*

$a > \rho_t$ Always $K_t > 1$

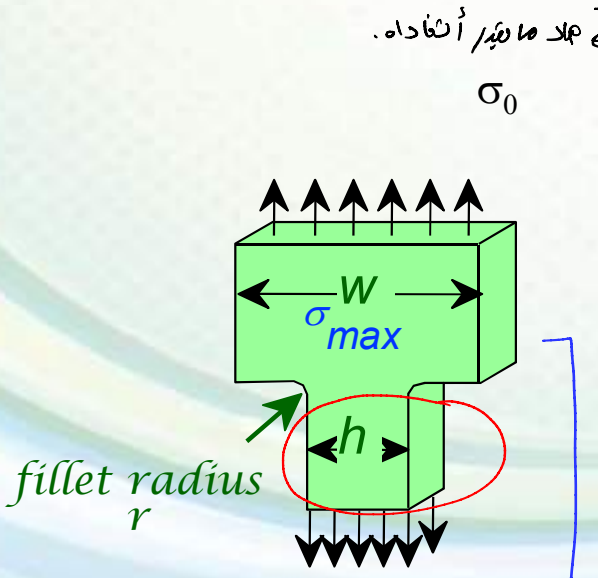
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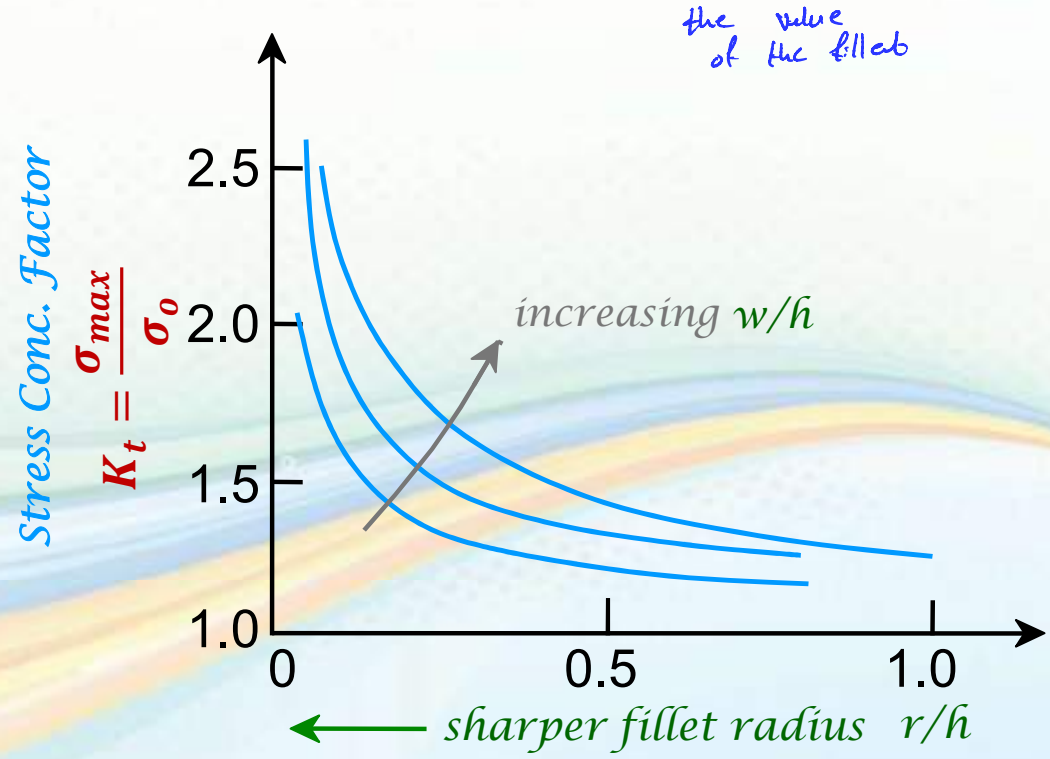
Engineering Fracture Design

- Avoid sharp corners

شخابات تقيد/ أتفادها عشان مايبقاش عندي crack على السطح internally أو

هلا ما تقيد/ أتفاداه.





Stress concentration factor depends on the value of the fillet

هون بيجاد التركيز لو إحنا صممنا fillets لما أثر بـ stress على minimum cross section Area عند failure المكوّن في بكون الـ

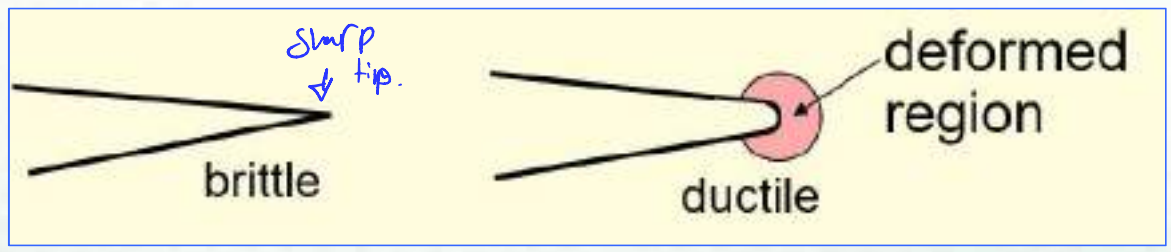
بين هو وفي بصير عند أكد العامل بيناتهو كانه إنتقلنا بسرعة من أعلى لأقل

stress مساحة الـ fillet في دور بعمل توزيع من سبب الـ

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Crack Propagation

- Cracks having sharp tips propagate easier than cracks having blunt tips
- A plastic material deforms at a crack tip, which "blunts" the crack.



Energy balance on the crack

- Elastic strain energy:
  - ✓ energy stored in material as it is elastically deformed
  - ✓ this energy is released when the crack propagates
  - ✓ creation of new surfaces requires energy

Criterion for Crack Propagation

- Crack propagates if crack-tip stress (σ_m) exceeds a critical stress (σ_c)

$$\sigma_c = \left(\frac{2E\gamma_s}{\pi a}\right)^{1/2}$$

- When the tensile stress at the tip of crack exceeds the critical stress value the crack propagates and results in fracture. (ductile + brittle)

where

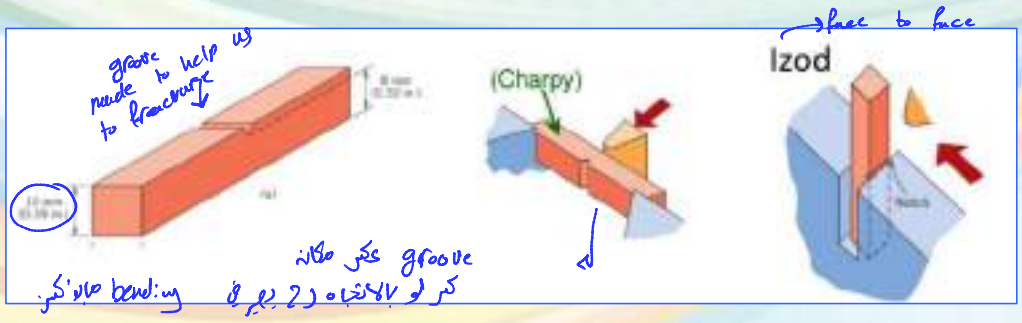
- E = modulus of elasticity
- γ_s = specific surface energy (elastic)
- a = one half length of internal crack

- For ductile materials ⟶ replace γ_s with $\gamma_s + \gamma_p$ (elastic + plastic)

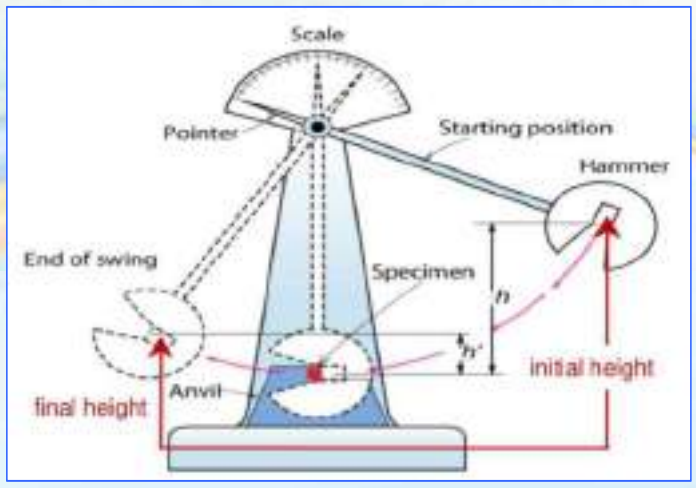
where γ_p is plastic deformation energy

Impact Fracture Testing → فحص مقاومة المعدن لقوة صدم مفاجئة

- *Impact tests are used in studying the toughness of material. A material's toughness is a factor of its ability to absorb energy during plastic deformation.* => fracture يعني كسر
- *Testing fracture characteristics under high strain rates.* (for ductile)
- *Two standard tests, the Charpy and Izod, measure the impact energy (the energy required to fracture a test piece under an impact load), also called the notch toughness*



كسر مكان groove
كسر لو بالاتجاه دا بيرجع



عندي هاد البندول بالبداية بحط لوزنة صغيرة و برميه وبحسب ارتفاع متى يوصل عشانة أحسب energy losses

قبل الاختبار زي الاحتكاك مع الهواء و المسنن .

بجيبن بهيب الـ load و بعمل الاختبار مع لوما الكبر بغيّر الوزنة .

لما أخيره والمؤشر الاختبار ويرجع بحسب كم اصغت طاقة .

load لما الحبة صار فيه كسر فقدت أحد ductile very

⊛ كمان مهم لازم أنبه إذا المادة

لما درجة الحرارة (درجة برودة الحبة) بتجربن بتنتقل عليها

وهيك كمان بتحمل لل brittle إذا كانت المرة بتذكر (بمعنى)

Ductile-to-brittle transition

(1)

- As temperature decreases a ductile material can become brittle - ductile-to-brittle transition

(2)

- Alloying usually increases the ductile-to-brittle transition temperature.

(*) كمبت أحوال المادة من Ductile لـ Brittle.

(3)

- FCC metals remain ductile down to very low temperatures.

(4)

- For ceramics, this type of transition occurs at much higher temperatures than for metals.
- The ductile-to-brittle transition can be measured by impact testing: the impact energy needed for fracture drops suddenly over a relatively narrow temperature range – temperature of the ductile-to-brittle transition.

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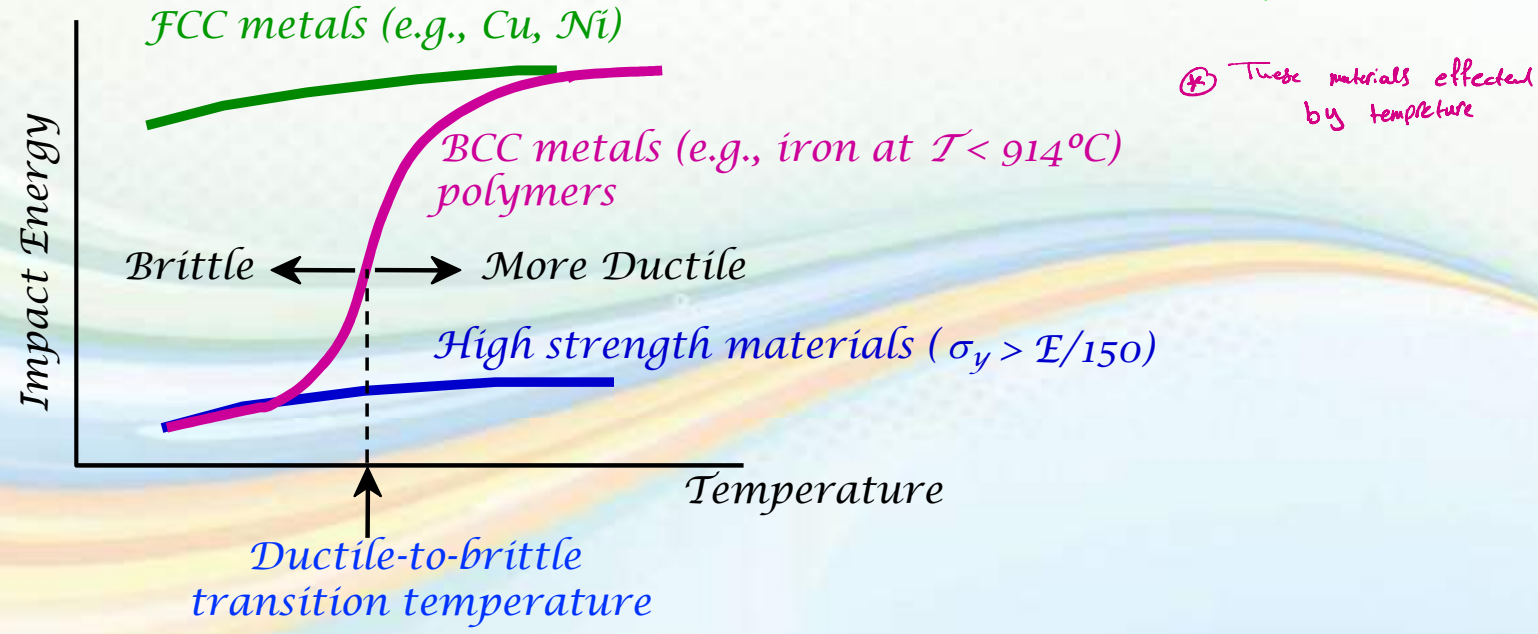
Influence of Temperature on Impact Energy

- Impact energy increases with increasing temperature to a point at which further increases in temperature do not cause a significant increase in impact energy

Ductile-to-Brittle Transition Temperature (DBTT)...

* low impact energy → brittle
* high impact energy → ductile

as we ↑ the T → they will remain Brittle, ductile



* These materials effected by temperature

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Design Strategy:

Stay Above The DBTT!

The Titanic



Liberty ships



- **Problem:** Steels were used having DBTT's just below room temperature.

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Fatigue

Failure under fluctuating / cyclic stresses

industrially ~ 55% failures are because of fatigue

- Under fluctuating / cyclic stresses, failure can occur at loads considerably lower than tensile or yield strengths of material under a static load: Fatigue.

not all materials will fracture under fatigue

- Estimated to causes 90% of all failures of metallic structures (bridges, aircraft, machine components, etc.)

* أغلب إنهيار أقل من الـ Ultimate وإنه عند أكثر من مرة Stress

- Fatigue failure is brittle like (relatively little plastic deformation) – even in normally ductile materials. Thus sudden and catastrophic.

=> ductile material with small reduction in cross sectional Area + No or a little elongation (Smooth surface) ↓ by fatigue.

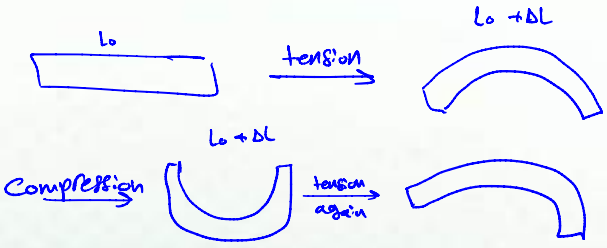
- Applied stresses causing fatigue may be axial (tension or compression), flextural (bending) or torsional (twisting).
- Fatigue failure proceeds in three distinct stages: crack initiation in the areas of stress concentration (near stress raisers), incremental crack propagation, final catastrophic failure.

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Fatigue: Cyclic Stresses I

- Cyclic stresses are characterized by maximum, minimum and mean stress, the range of stress, the stress amplitude, and the stress ratio.

1- Mean stress: $$\sigma_m = \frac{\sigma_{max} + \sigma_{min}}{2}$$



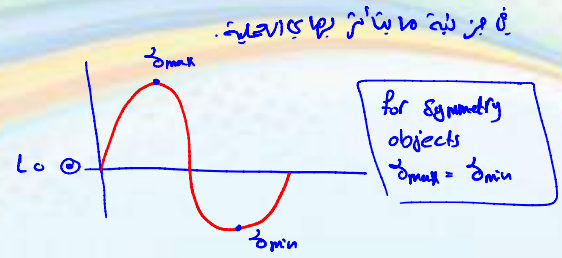
2- Range of stress: $$\sigma_r = \Delta\sigma = \sigma_{max} - \sigma_{min}$$

3- Stress amplitude: $$\sigma_a = \frac{\sigma_r}{2} = \frac{\sigma_{max} - \sigma_{min}}{2}$$

↳ equal to zero if we have symmetry

4- Stress ratio: $$R = \frac{\sigma_{min}}{\sigma_{max}}$$

↳ equal to one if we have symmetry



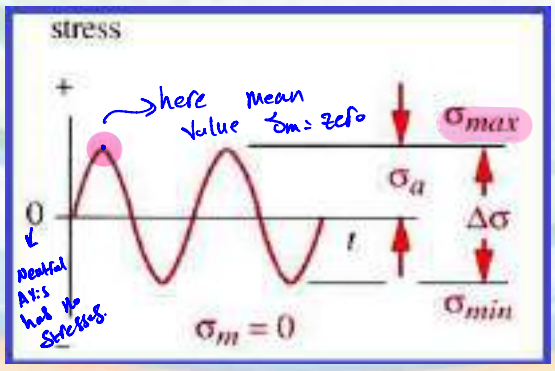
- Remember the convention that tensile stresses are positive, compressive stresses are negative.

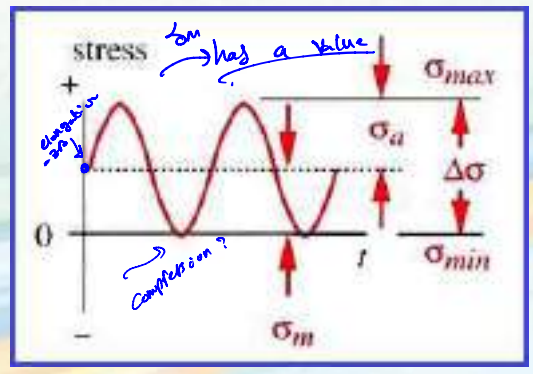
Fatigue: Cyclic Stresses II

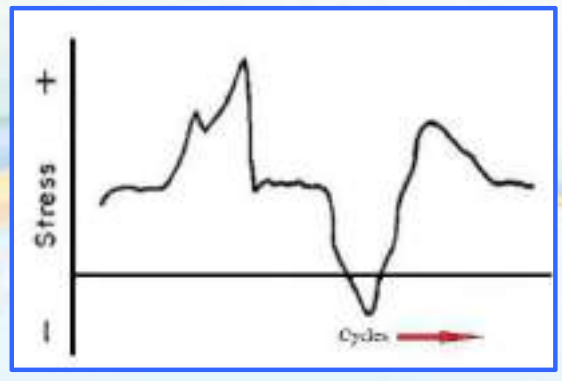
1- **Reversed stress cycle:** the stress alternates from a maximum tensile stress to a maximum compressive stress of equal magnitude

2- **Repeated stress cycle:** maximum and minimum stresses are asymmetrical relative to the zero stress level

3- **Random stress** fluctuation







- Alternating stress $\sigma_a = \frac{\sigma_{max} - \sigma_{min}}{2}$
- Mean stress $\sigma_m = \frac{\sigma_{max} + \sigma_{min}}{2}$

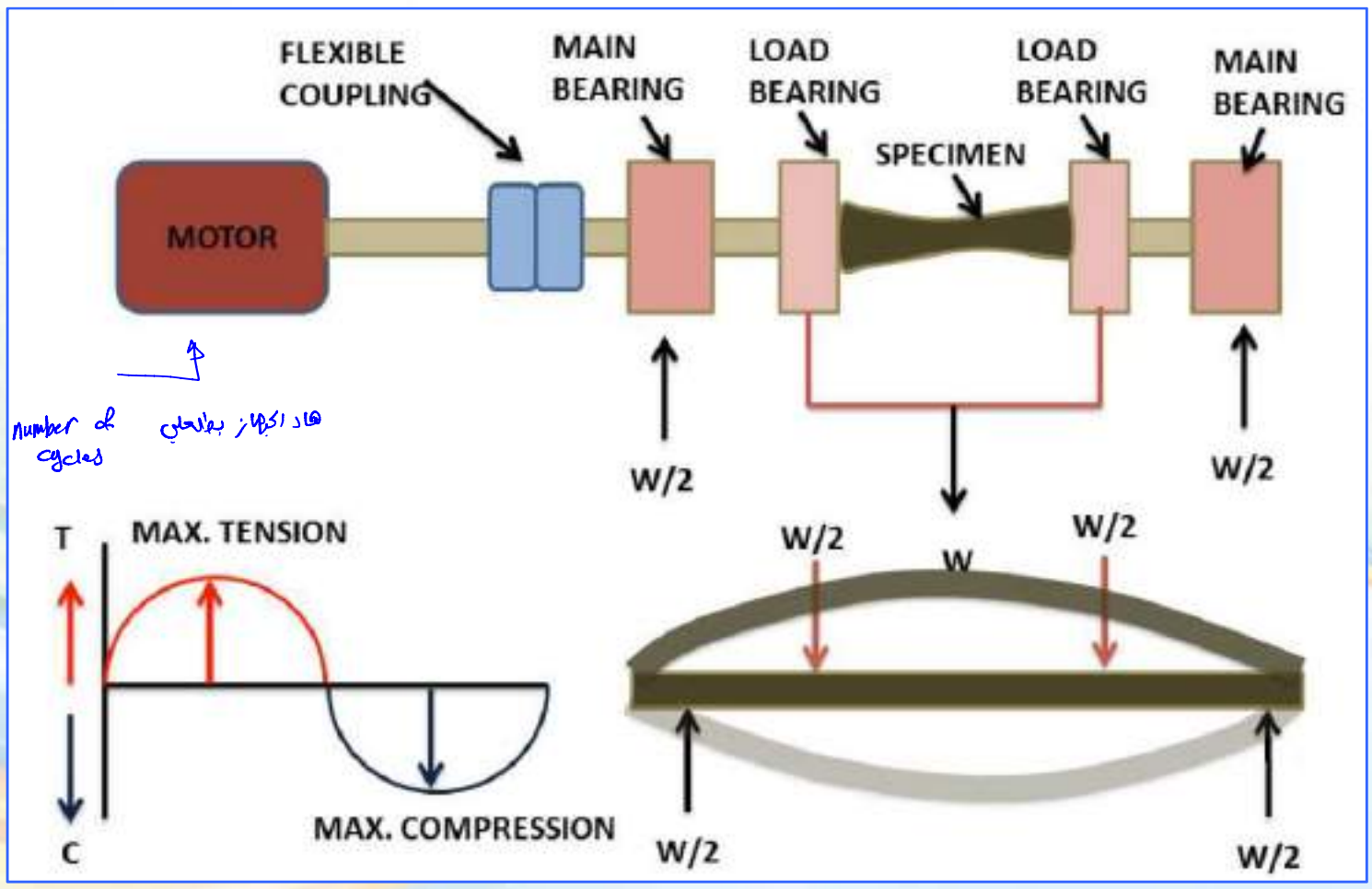
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هون عنا الجسّة معمولة load ثابت وبتخلّيها دايمًا tension لحالها بدون تعمل tension والمادة بتفوق لهذه الـ load أكتر المساحة هي الجسّة بدّير compression بدل ما تكسر.. ح باختصار لفات وبجي عند هاد الـ load بدّي أعرف كم مرة لازم أعمل له (مثلًا) 3 مليون لفة كاملة ح one complete cycle

لفة كاملة ح
↓
tension + compression

لازم أعرف كم مرة لازم أعمل له load هاد الجهاز بعالجي number of cycles

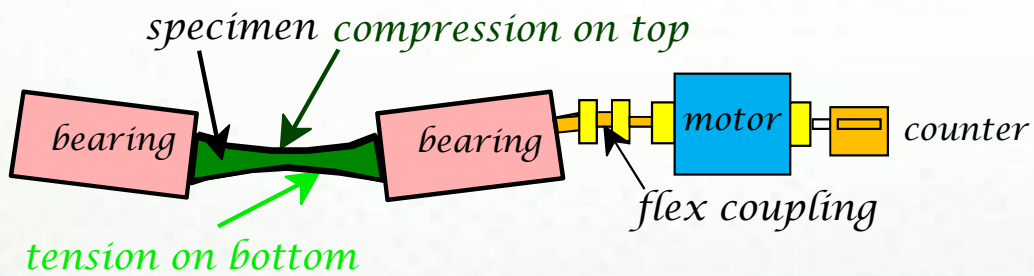
load ↑ number of cycles ↓



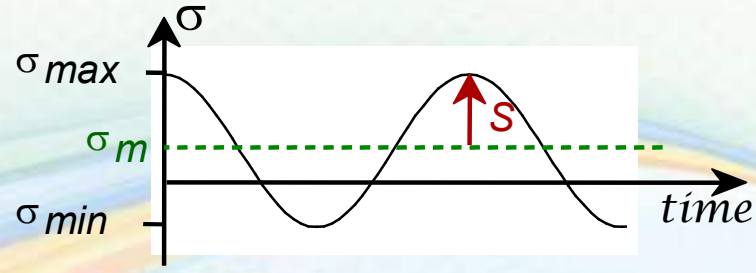
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Fatigue

- **Fatigue** = failure under applied cyclic stress.



- Stress varies with time.
  - Key parameters are S, σ_m, and cycling frequency

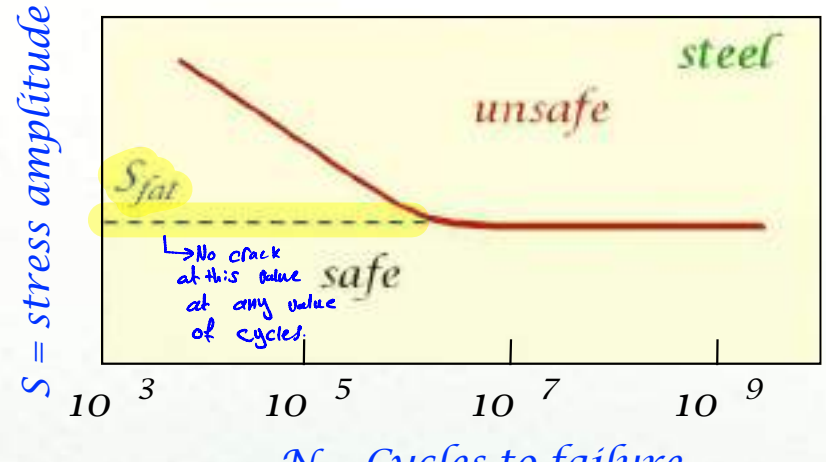


- Key points: Fatigue...
  - Can cause part failure, even though $\sigma_{max} < \sigma_c$.
  - Responsible for ~ 90% of mechanical engineering failures.

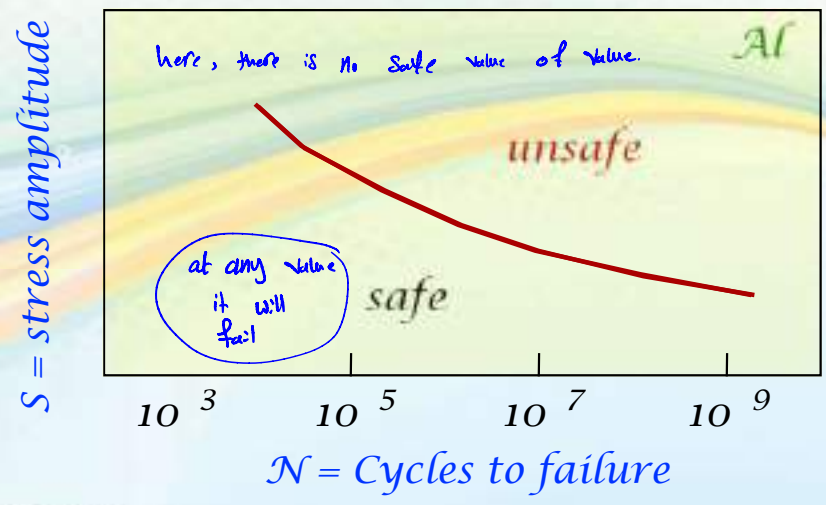
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Types of Fatigue Behavior

- Fatigue limit, S_{fat}:
  - no fatigue if $S < S_{fat}$



- For some materials, there is no fatigue limit!



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Rate of Fatigue Crack Growth

Fatigue
→ 1) flaw
2) crack formation
3) growth of crack
↓ slow ductile
↓ fast Brittle

- Crack grows incrementally

$$\frac{da}{dN} = (\Delta K)^m \sim (\Delta\sigma)\sqrt{a}$$

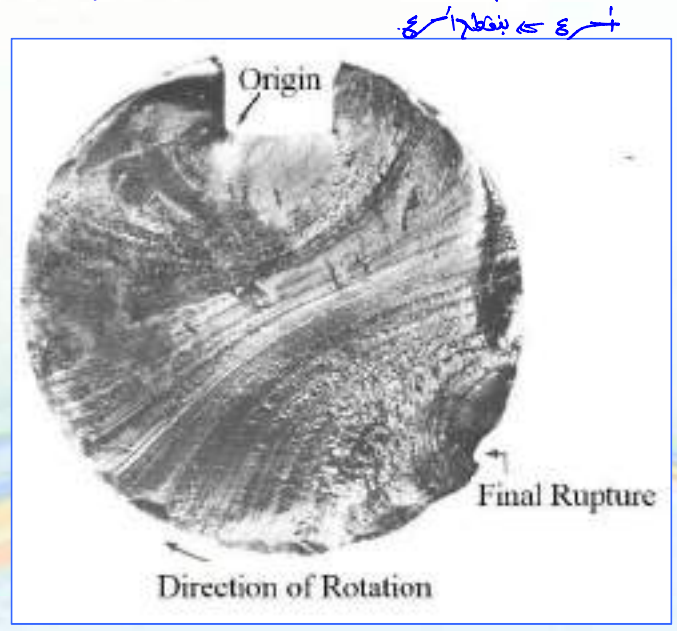
typ. 1 to 6

m higher ⇒ more brittle.

a = length of the crack

increase in crack length per loading cycle

Loading frequency ↑
crack propagation is faster
زيادة التردد بالسالب
سرعة ⇐ بتقلل السرعة



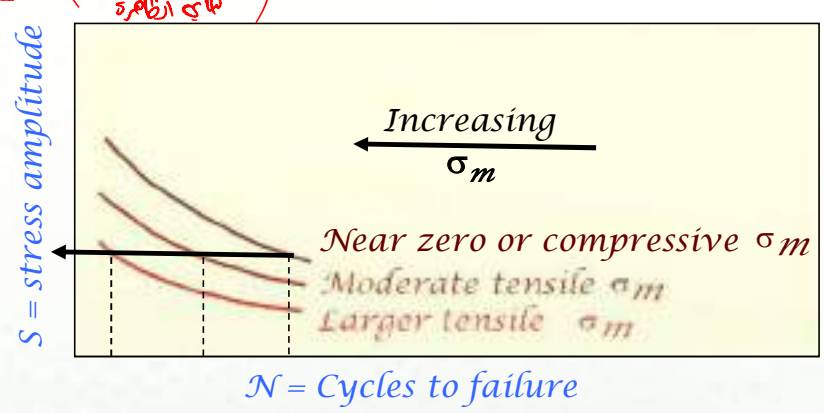
- Failed rotating shaft
  - Crack grew even though $K_{max} < K_c$
  - Crack grows faster as
    - ✓ $\Delta\sigma$ increases
    - ✓ Crack gets longer
    - ✓ Loading freq. increases.

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Improving Fatigue Life

improving => (تحسين / زيادة / عمر / التعب)

1. Impose compressive surface stresses (to suppress surface cracks from growing)

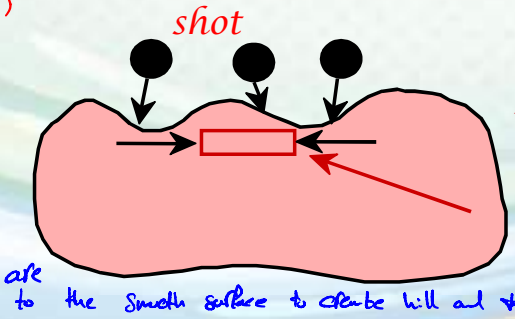


when surface of metal is smooth

So when we apply force (tension, compression) all the surface will be under this force

=> so to decrease the effect this forces by shot peening

Method 1: Shot peening



very small solid particles are shot in very fast speed to the smooth surface to create hill and valleys

also to create tension + compression, we will elimate cyclic stresses.

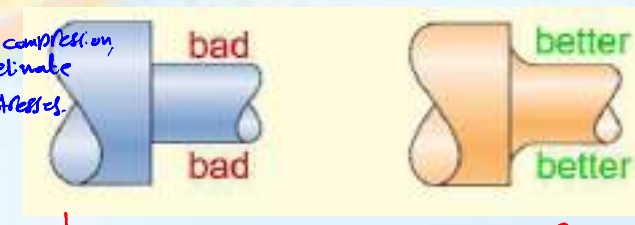
(delay of fracture) by increase number of cycles

Method 2: Carburizing



زيادة كربون أعلى كثافة للسطح حالي يزيد لـ

2. Remove stress concentrators.



We can improve this sample's fatigue life by avoiding sharp corners

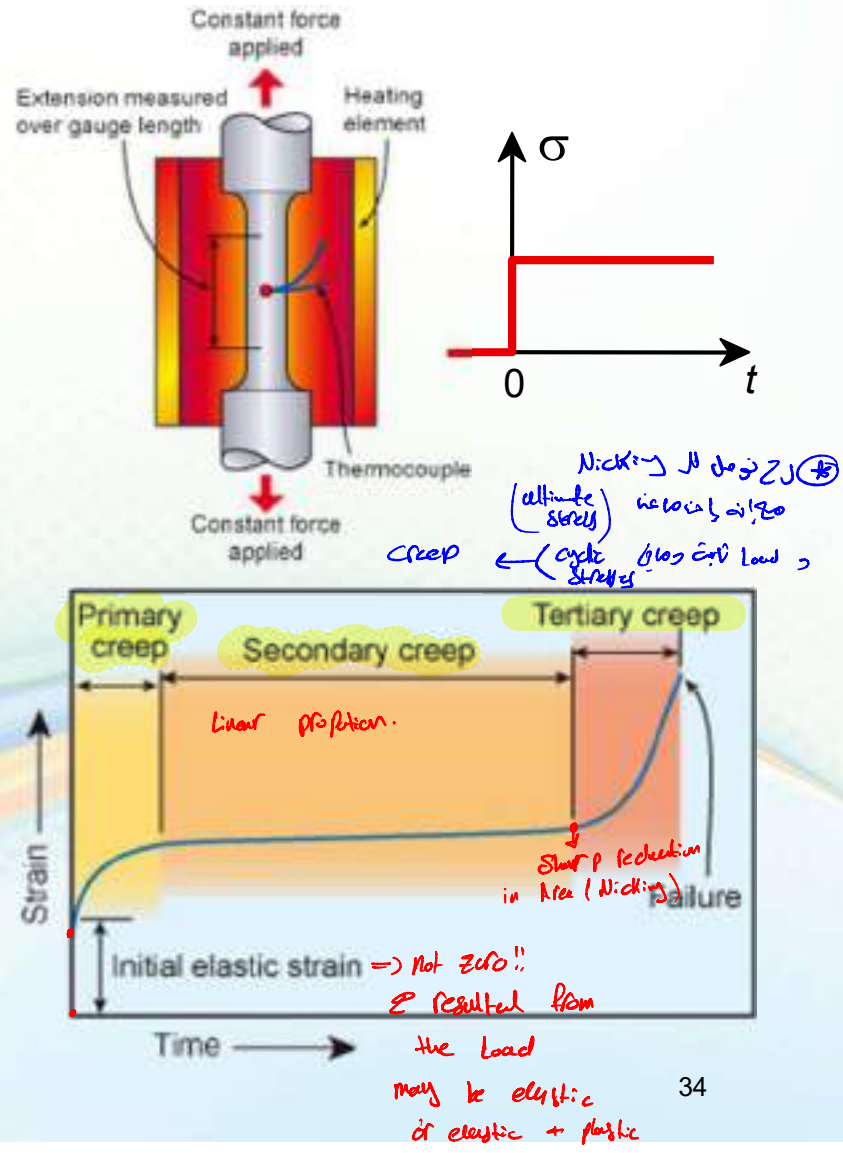
So, by design, we'll do this fillet => gradual transfer of Area.

Yousef Muharak
Material Science
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Creep

- Creep testing is conducted using a tensile specimen to which a constant stress is applied at a constant temperature, often by the simple method of suspending weights from it.
- The test is recorded on a graph of strain versus time. Sample deformation at a constant stress (s) vs. time

1. **Primary Creep:** slope (creep rate) decreases with time.
2. **Secondary Creep:** steady-state, i.e., constant slope ($\Delta\varepsilon/\Delta t$).
3. **Tertiary Creep:** slope (creep rate) increases with time, i.e. acceleration of rate.

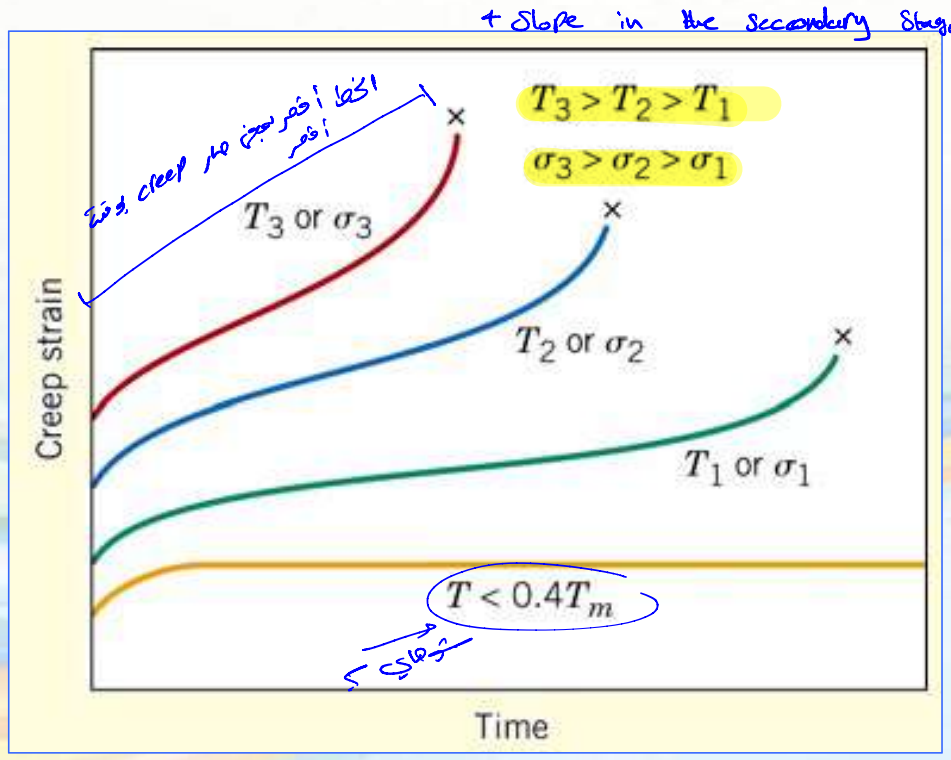


I can increase rate of strain (creep) by increasing time

Creep: Temperature Dependence

- *Occurs at elevated temperature, $T > 0.4\,T_m$ (in K)*

+ slope in the secondary stage will ↑



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Secondary Creep

- Strain rate is constant at a given T, σ.

stress exponent (material parameter)

$$\dot{\varepsilon}_s = K_2 \sigma^n exp\left(\frac{-Q_c}{RT}\right)$$

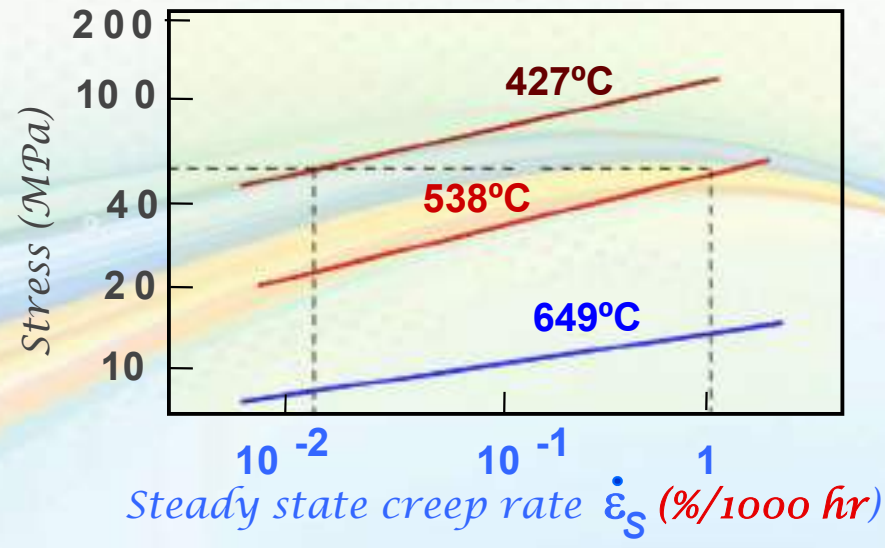
strain rate

material const.

applied stress

activation energy for creep (material parameter)

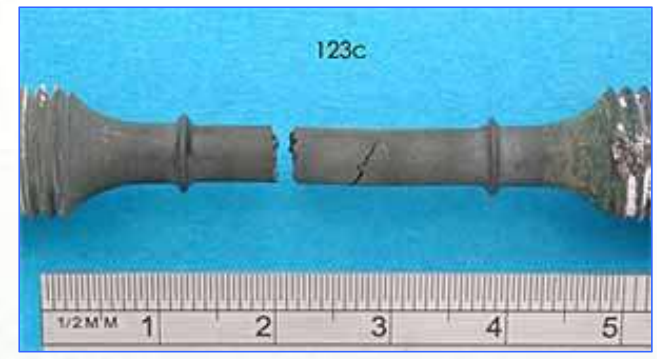
- Strain rate increases with increasing T, σ



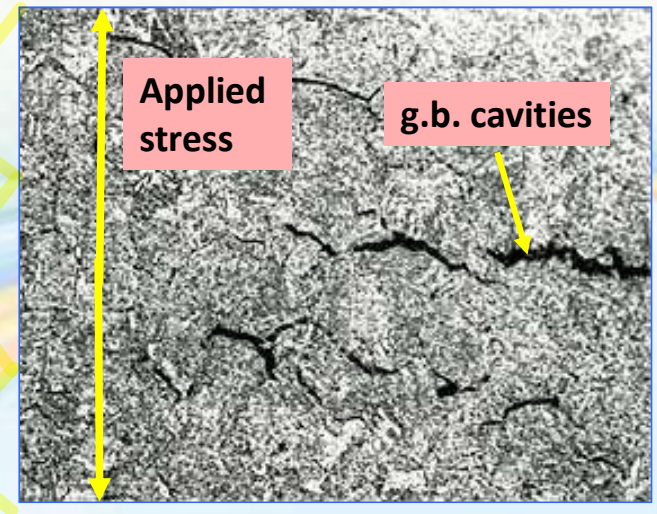
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Creep Failure

- Failure: voids that form on the grain boundaries in the early stages of creep.







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Prediction of Creep Rupture Lifetime

- Estimate rupture time of S-590 Iron at $T = 800°C$ and a stress value of 20,000 psi

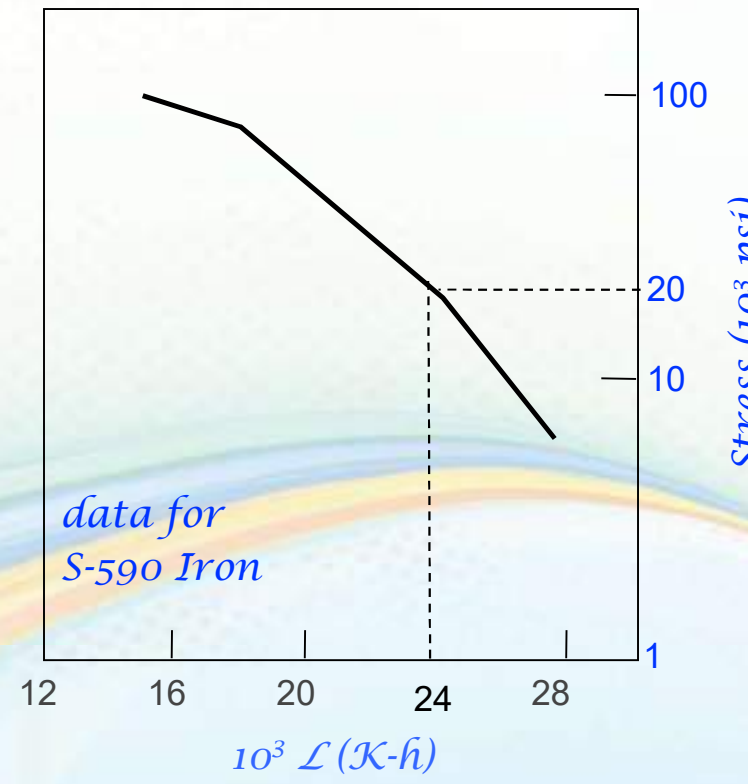
- **Time to rupture, t_r**

$$T(20 + \log t_r) = L$$

Temperature — Time to failure (rupture) — Function of applied stress

$$(1073\ K)(20 + \log t_r) = 24 \times 10^3$$

Ans: $t_r = 233\ hr$



$\mathcal{L}$: Larson–Miller parameter

Prediction of Creep Rupture Lifetime

- Estimate rupture time of S-590 Iron at $T = 750°C$ and a stress value of 20,000 psi

نزلنا درجة الحرارة فحيل
و الأثر كمان عالي

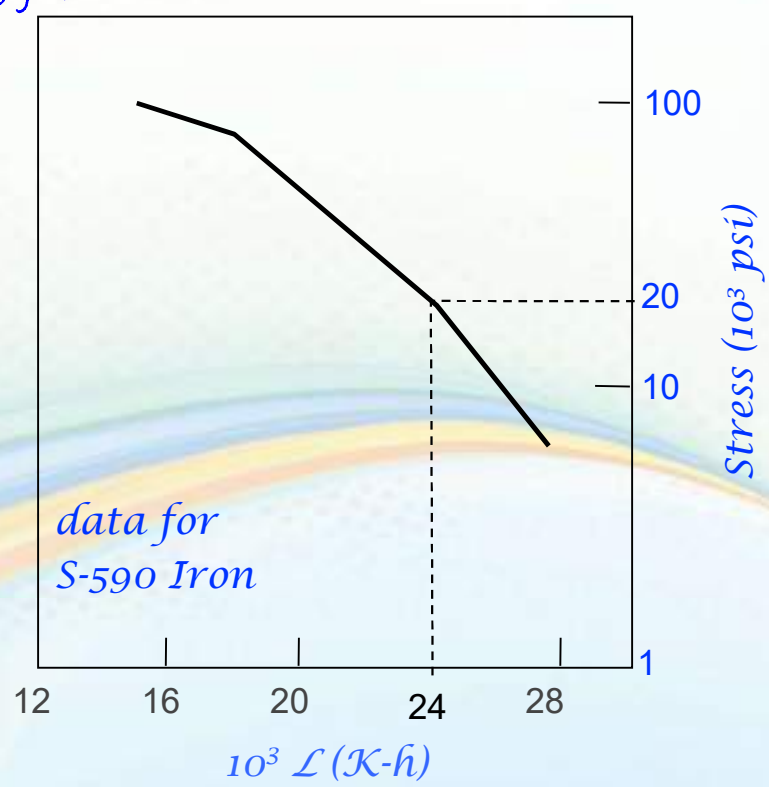
- **Time to rupture, t_r**

$$T(20 + \log t_r) = L$$

Temperature — Time to failure (rupture) — Function of applied stress

$$(1023\ K)(20 + \log t_r) = 24 \times 10^3$$

Ans: $t_r = 2890\ hr$



microcracks → propagation at tips will increase because of stress concentration there → failure

ductile ⇒ crack @ grain boundaries

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SUMMARY

- Engineering materials not as strong as predicted by theory.
- Flaws act as stress concentrators that cause failure at stresses lower than theoretical values.
- Sharp corners produce large stress concentrations and premature failure.
- Failure type depends on T and σ:
  - For simple fracture (noncyclic σ and $T < 0.4T_m$), failure stress decreases with:
    - ✓ Increased maximum flaw size,
    - ✓ Decreased T,
    - ✓ Increased rate of loading.
  - For fatigue (cyclic σ):
    - ✓ Cycles to fail decreases as $\Delta\sigma$ increases.
  - For creep ($T > 0.4T_m$):
    - ✓ Time to rupture decreases as σ or T increases.

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Chapter 7

Phase Diagrams

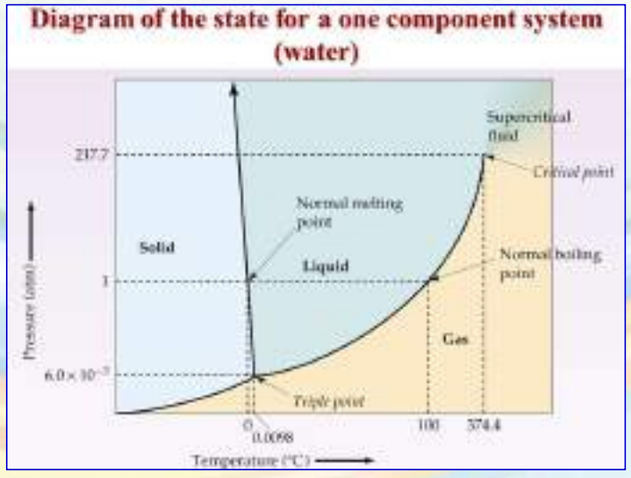
The University of Jordan
Chemical Engineering Department
First Semester 2021
Prof. Yousef Mubarak

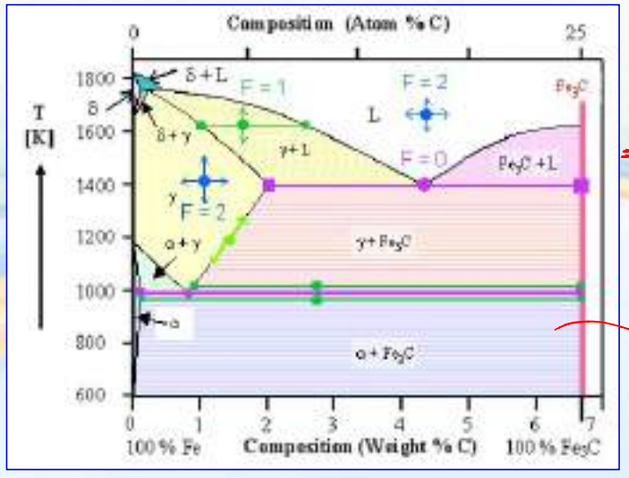
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Chapter 7

Phase Diagrams

graphical representation of the two or more component in more than state or phase and how it will change @ given (T, P, composition)





⇒ number of the States
↳ ② ↳ Liquid
↳ Solid

2 phases in one Solid State

Yousef Muharak
Materials Science

@ if there is one microstate (one phase) here the phase is the state also such as ice.

phase vs State

State ⇒ one more than phase
(مكون)
(طور و حالة غاز)

phase ⇒ microstate structure in one State @ have different properties
زي أشكال الكربيد ة في الحالة الصلبة
أو سمات تركيبية

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ISSUES TO ADDRESS...

- When we combine two elements...

  what is the resulting equilibrium state?

- In particular, if we specify...
  - the composition (e.g., wt% Au - wt% Pb), and
  - the temperature (T)

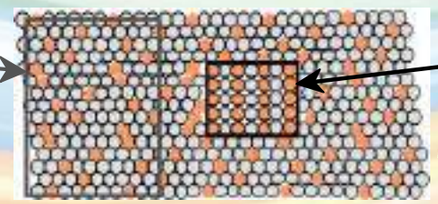
then...

- How many phases form?
- What is the composition of each phase?
- What is the amount of each phase?

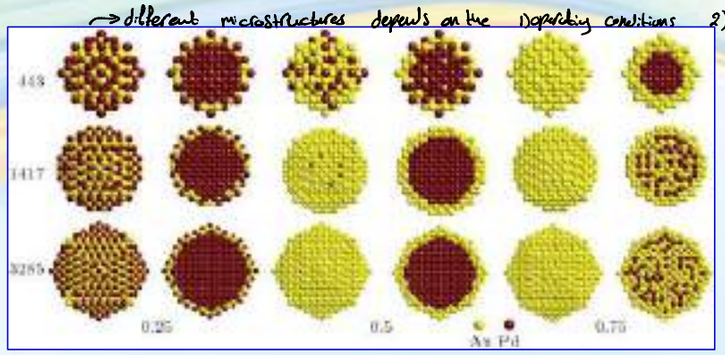
Phase A (random distribution) → Pb

Phase B

phase A has completly different property from phase B



○ Au atom
● Pb atom



different microstructures depends on the 1)parting conditions 2)composition

Outline

- Definitions and basic concepts.
- Phases and microstructure
- Binary isomorphous systems (complete solid solubility)
- Binary eutectic systems (limited solid solubility)
- Binary systems with intermediate phases/compounds
- The iron-carbon system (steel and cast iron)

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Definitions: Components and Phases

- **Component:** chemically recognizable species (Fe and C in carbon steel, H_2O and NaCl in salted water). ⇒ عنصر او مركب كيميائي
- A binary alloy contains two components, a ternary alloy – three, etc. Number of compants will dedict the name of the system
- **Phase:** a portion of a system that has uniform physical and chemical characteristics. ⇒ micro structure in one Solid State — one more than microstructures → different properties.
- Two distinct phases in a system have distinct physical or chemical characteristics (e.g. water and ice) and are separated from each other by definite phase boundaries.

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Definitions: Components and Phases

- A phase may contain one or more components. such as carbon in iron
- A single-phase system is called homogeneous, systems with two or more phases are mixtures or heterogeneous systems.

Composition of cementite in (2) > (1)



(1) Also different distribution

Perlite: ferrite and cementite

in these pictures, All of them are perlite but with different composition of cementite & different operating conditions.

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Definitions: Solubility Limit

- *Solvent:* host or major component in solution.
- *Solute:* minor component.
- *Solubility Limit* of a component in a phase is the maximum amount of the component that can be dissolved in it (e.g. alcohol has unlimited solubility in water, sugar has a limited solubility, oil is insoluble).
- The same concepts apply to solid phases: Cu and Ni are mutually soluble in any amount (unlimited solid solubility), while C has a limited solubility in Fe.

Solubility in metal
⇒ will combine and disperse in the molten state





Question:

What is the solubility limit for sugar in water at 20°C?

Answer:

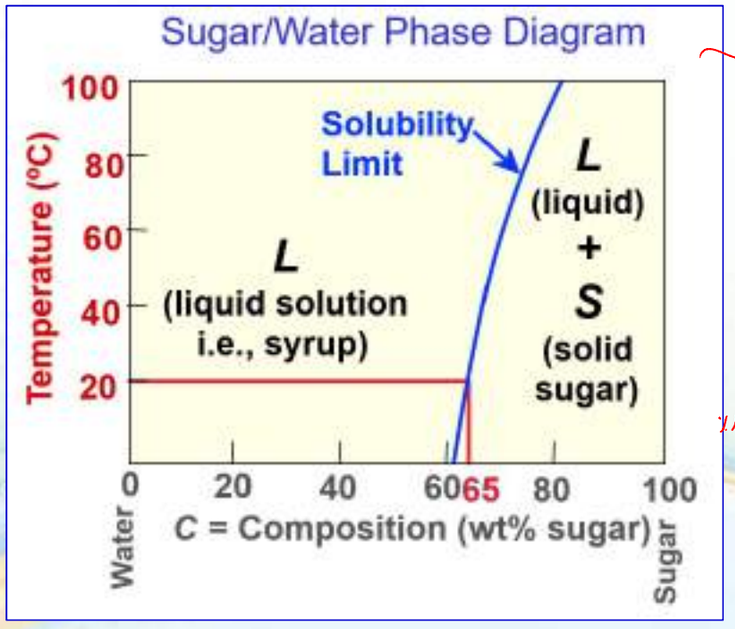
65 wt% sugar.

At 20°C, if C < 65 wt% sugar:

syrup

At 20°C, if C > 65 wt% sugar:

syrup + sugar



Solubility ۸ ح
ت ۸

لو هنتے ٪۶۵ سکر ی ۲۰°ح
ل ذوب
بس لو هنتے ٪۸۰ ی فضی
درجة الحرارة ل ذوب
٪۶۵ ت ل ذوب ویضل ٪۱۵

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Microstructure

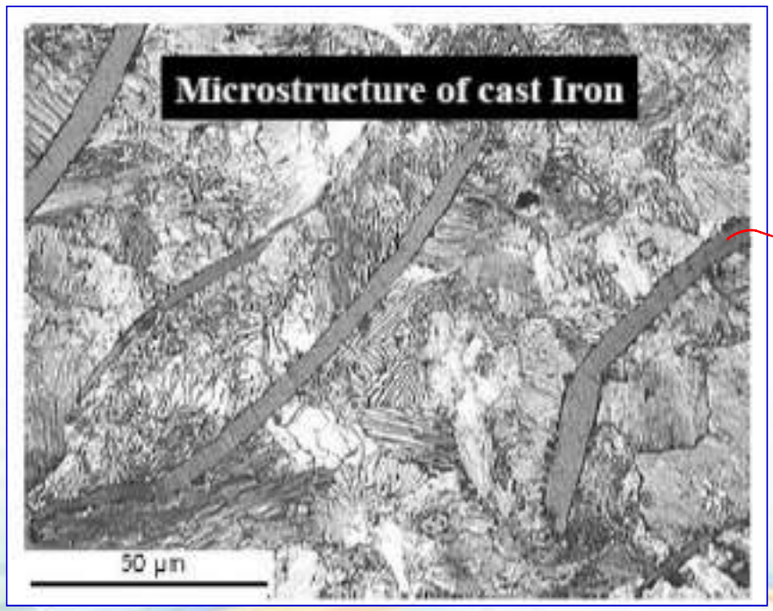
- The properties of an alloy depend not only on proportions of the phases but also on how they are arranged structurally at the microscopic level. ⇒ على مستوى مجهري
- Thus, the microstructure is specified by:

1. The number of phases,
2. Their proportions, (composition)
3. And their arrangement in space.

→ we can predict Thermal, optical etc. properties.

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- This is an alloy of Fe with 4 wt.% C.
- There are several phases. The long gray regions are flakes of graphite. The matrix is a fine mixture of BCC Fe and Fe_3C compound.



- Phase diagrams will help us to understand and predict the microstructures like the one shown in this photo.

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Equilibrium and Metastable States

- A system is at equilibrium if at constant temperature, pressure and composition the system is stable, not changing with time.
- Equilibrium is the state that is achieved given sufficient time.

equilibrium → we mean by (final stage) → No change at all with time

- But the time to achieve equilibrium may be very long (the kinetics can be slow) that a state along the path to the equilibrium may appear to be stable.
- This is called a metastable state.

↳ Not reach the final stage

لحزي كانه شد بده يطلع درجه الحراره ولا يرتاح

على السطح هون السطح هو الـ equilibrium بس أثناء الـ heat

Metastable حزرد يرتاح بالطاقه الثالث فهون صار

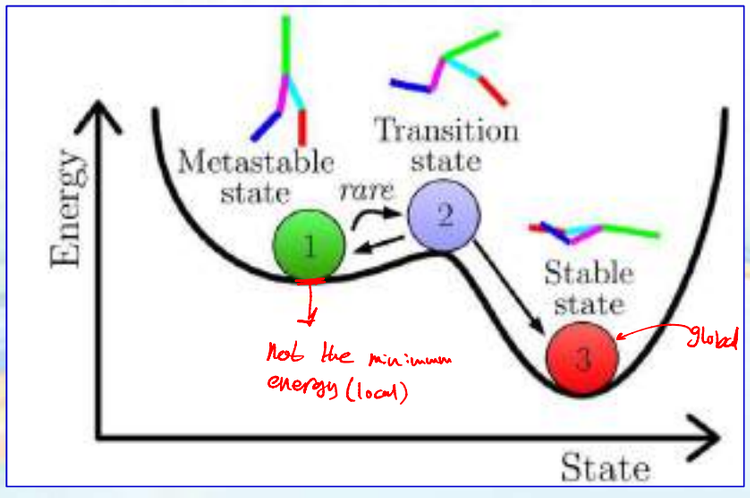
نفس سي اعواد

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Equilibrium and Metastable States

- In thermodynamics, equilibrium is described as the state of system that corresponds to the minimum of the thermodynamic function called the free energy of the system.

- Free energy is a function of the internal energy of a system, and also the randomness or disorder of the atoms or molecules (or entropy)



Equilibrium and Metastable States

Thermodynamics tells us that:

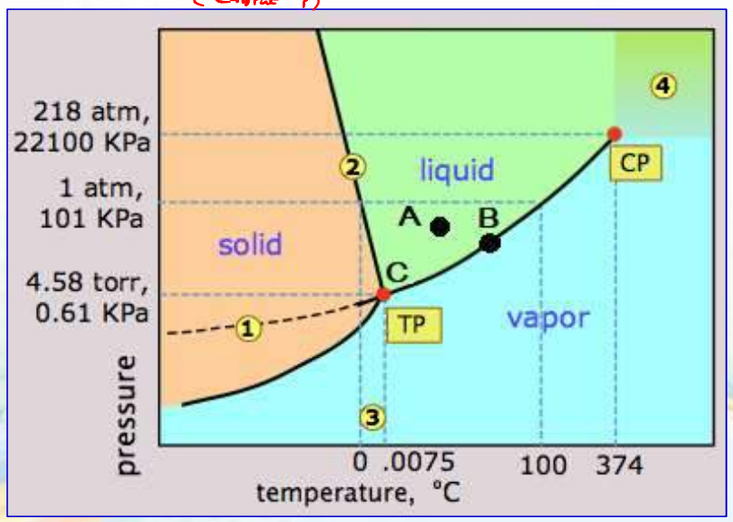
- Under conditions of a constant temperature and pressure and composition, the direction of any spontaneous change is toward a lower free energy.
- The state of stable thermodynamic equilibrium is the one with minimum free energy.
- A system at a metastable state is trapped in a local minimum of free energy that is not the global one.

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Phase diagram

- A phase diagram: graphical representation of the combinations of temperature, pressure, composition, or other variables for which specific phases exist at equilibrium.
- For H_2O, a typical diagram shows the temperature and pressure at which ice (solid), water (liquid) and steam (gas) exist.

All Alloys phase diagrams @ atmospheric pressure (Constant P)



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Phase diagram

- A phase diagrams show what phases exist at equilibrium and what phase transformations we can expect when we change one of the parameters of the system (T, P, composition).
- We will discuss phase diagrams for binary alloys only and will assume pressure to be constant at one atmosphere.
- Phase diagrams for materials with more than two components are complex and difficult to represent.

Metastable vs equilibrium

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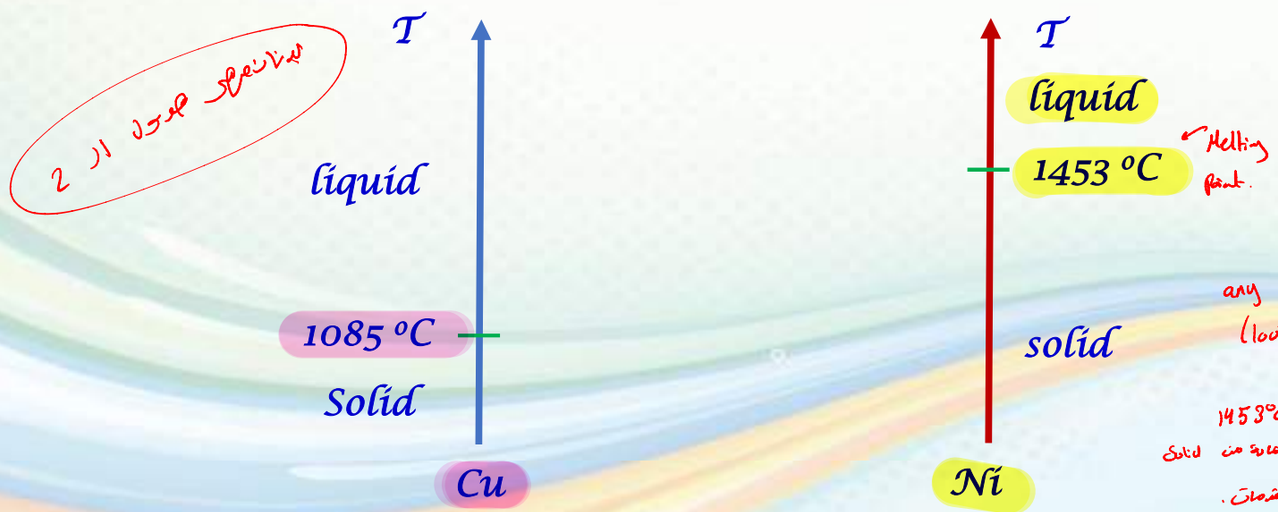


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1- Unary System ⇒ one component only

- Consider 2 elemental metals separately:
  - Cu has melting $T = 1085\ ^oC$
  - Ni has melting $T = 1453\ ^oC$

(at standard $P = 1$ atm)



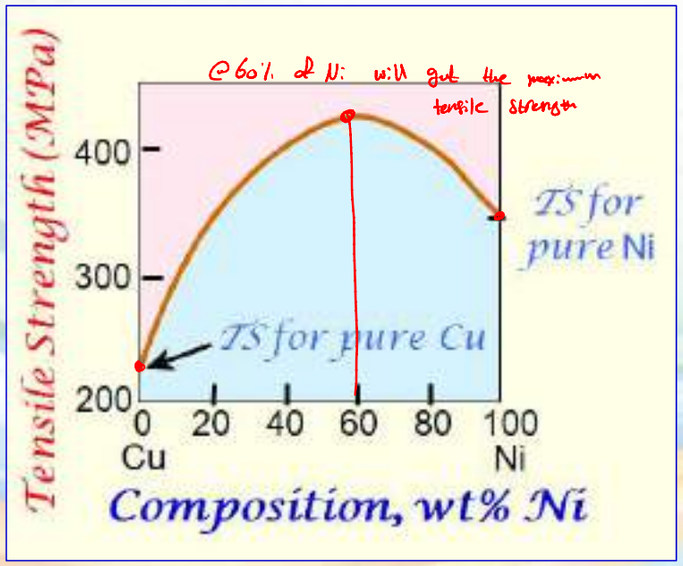
- What happens when Cu and N are mixed?

Why Alloys?

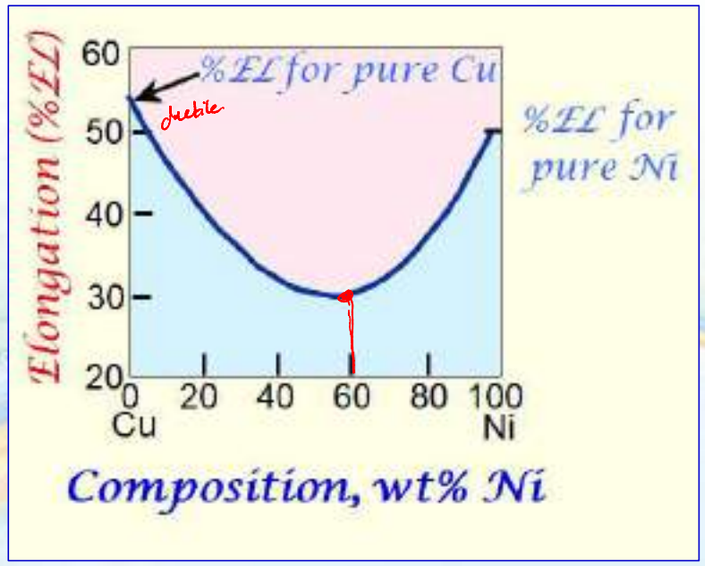
mixing two or more metal.

- Effect of solid solution strengthening on:

-- Tensile strength (TS)



-- Ductility (%EL)



Ni: من 60٪ هنا جو إحنا جو هنا
Tensile strength حسينا من
ductility بالمقابل قللنا
نتيجة هاي اضافة
عند نقص الكمية
الفكرة هي حسب التكلفة والاستخدام
لـ أجهز الـ alloy

لما أخلط كمية معينة مهم
على أي درجة حرارة رح تذوب؟
لـ ذكونة بها

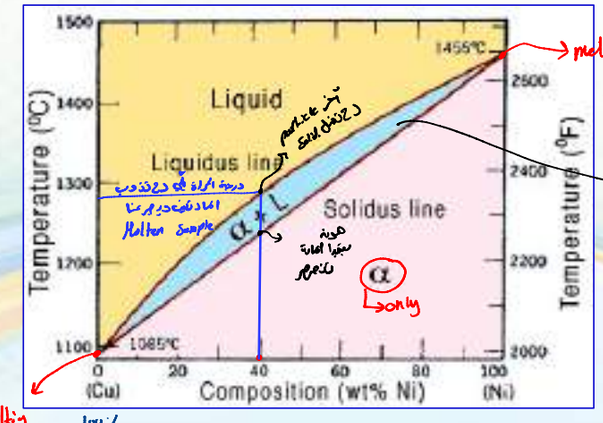
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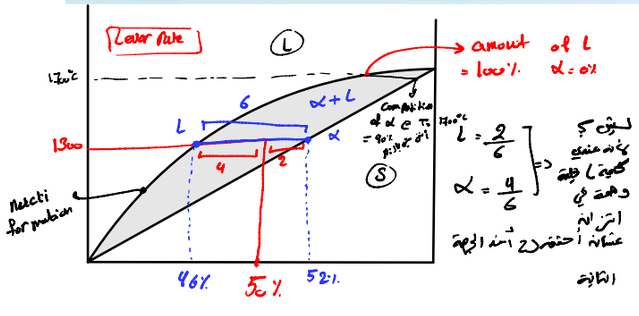
2- Binary Isomorphous Systems

- **Isomorphous system:** (solid solution) complete solid solubility of the two components (both in the liquid and solid phases).

- Three phase region can be identified on the phase diagram:

1. Liquid (L) , solid + liquid (α +L), solid (α)
2. Liquidus line separates liquid from liquid + solid
3. Solidus line separates solid from liquid + solid.





Lever rule is applicable only if we have two or more than one phase

What is the composition of α, L?

- α = 52%
- L = 46%

(α+L) => metastable zone because at any T (in this range) α and L comp will change to know the amount of α and L is by Lever rule at T => (α +L) in equilibrium

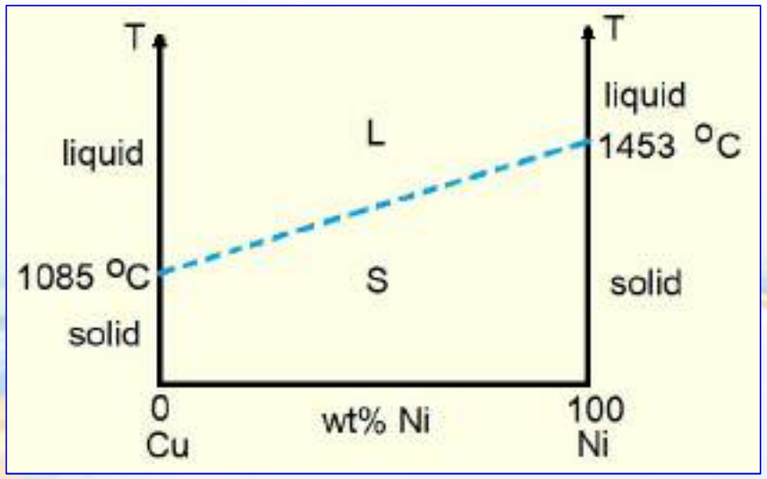
What is the weight fraction of α? @ T = 900°C (100%) => only one structure.

Binary Isomorphous Systems

- Binary: 2 components
- Isomorphous: complete liquid and solid solubility ⇒ No limitation in Solubility

✓ Expect T_m of solution to lie between T_m of two pure components.

✓ For a pure component, complete melting occurs before T increases (sharp phase transition). But for multicomponent system, there is usually a coexistence of L and S.



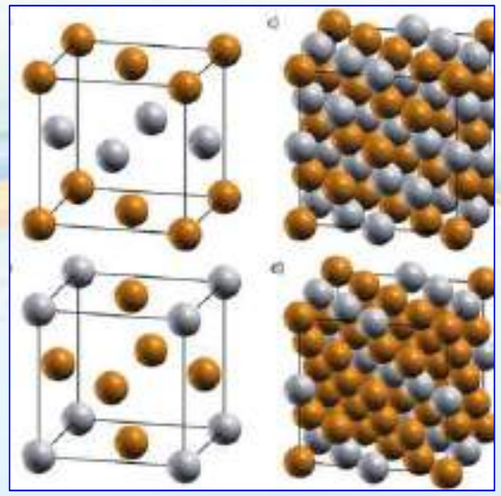
Binary Isomorphous Systems

- Example of isomorphous system Cu-Ni
- The complete solubility occurs because:
  1. Both Cu and Ni have the same crystal structure, FCC
  2. Similar radii
  3. Electronegativity
  4. Valence



Characteristics of Selected Elements

Element	Symbol	Atomic Number	Atomic Weight (amu)	Density of Solid, 20°C (g/cm³)	Crystal Structure, 20°C	Atomic Radius (nm)	Ionic Radius (nm)	Most Common Valence
Cobalt	Co	27	58.93	8.9	HCP	0.125	0.072	2+
Copper	Cu	29	63.55	8.94	FCC	0.128	0.096	1+
Fluorine	F	9	19.00	—	—	—	0.133	1−
Gallium	Ga	31	69.72	5.90	Ortho.	0.122	0.062	3+
Neon	Ne	10	20.18	—	—	—	—	Inert
Nickel	Ni	28	58.69	8.90	FCC	0.125	0.069	2+
Niobium	Nb	41	92.91	8.57	BCC	0.143	0.069	5+



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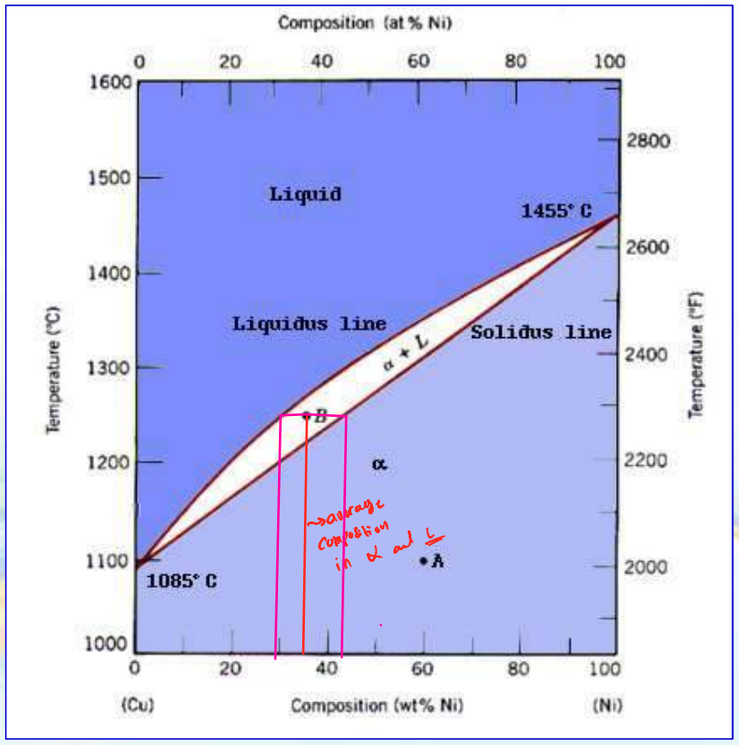
Binary Isomorphous Systems

What can we learn from this phase diagram?

1. Phase(s) present.
   - ✓ A: solid (α) only
   - ✓ B: solid and liquid
2. Composition of those phases
   - ✓ A: 60 wt% Ni
   - ✓ B: 35 wt% Ni overall (how about in L and S separately?)
3. Amount of the phases.
   - ✓ A: 100 % α phase
   - ✓ B: % solid and % liquid?

↳ by lever rule

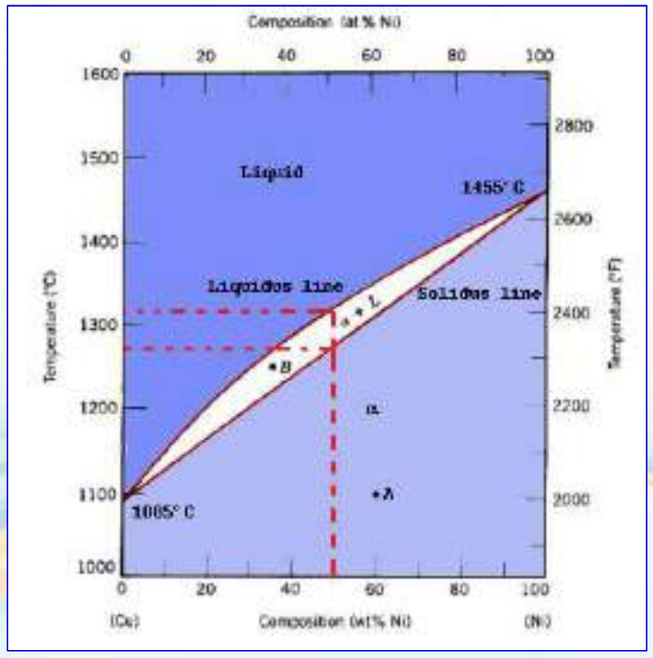
α +



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Binary Isomorphous Systems

- In one-component system melting occurs at a well-defined melting temperature. ⇒ Sharp melting point
- In multi-component systems melting occurs over the range of temperatures, between the solidus and liquidus lines.
- Solid and liquid phases are in equilibrium in this temperature range.



Interpretation of Phase Diagrams

- *For a given temperature and composition we can use phase diagram to determine:*
  - *1) The phases that are present*
  - *2) Compositions of the phases*
  - *3) The relative fractions of the phases*
- *Finding the composition in a two phase region:*
  - *1) Locate composition and temperature in diagram.*
  - *2) In two phase region draw the tie line or isotherm.*
  - *3) Note intersection with phase boundaries. Read compositions at the intersections.*
- *The liquid and solid phases have these compositions.*

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Determining phase composition

Consider C_o = 35 wt% Ni

At T_A = 1320°C: Only Liquid (L) present

$C_L = C_o$ (= 35 wt% Ni)

At T_D = 1190°C: Only Solid (α) present

$C_\alpha = C_o$ (= 35 wt% Ni)

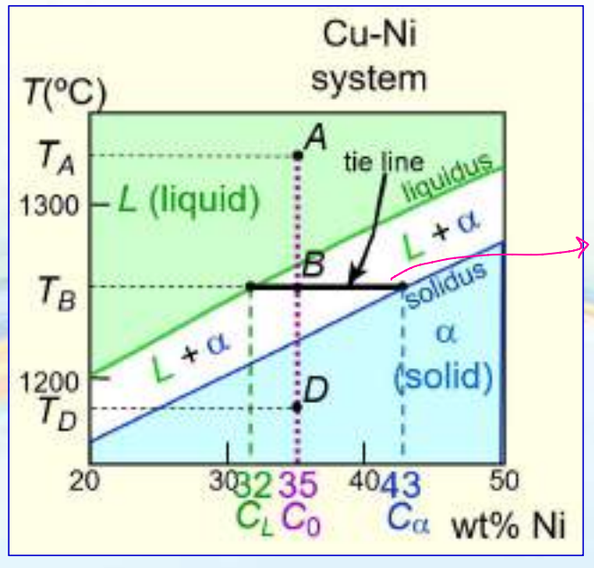
Determining phase composition in 2-phase region

1- At 1250 °C, draw the tie line.

2- Note where the tie line intersects the liquidus and solidus lines (i.e. where the tie line crosses the phase boundaries).

3- Read off the composition at the boundaries:

- ✓ Liquid is composed of CL amount of Ni (32 et% Ni)
- ✓ Solid is composed of Ca amount of Ni (43 wt% Ni)



صحيح بالنظر أعرف amount of solid و liquid لما Solid في ½ Liquid في ½ يعني كم هيتجزئ دنا سايبها بحسب

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Determination of phase weight fractions

- *If there is only one phase, then the weight fraction of either solid or liquid will be 100 wt%*

- *Examples:*

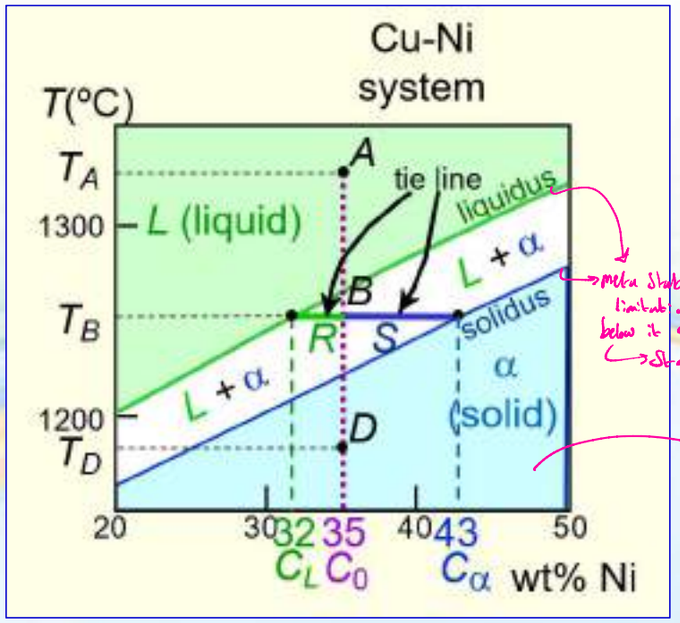
Consider C_0 = 35 wt% Ni

At T_A: Only Liquid ($\mathcal{L}$) present

$W_{\mathcal{L}}$ = 1.00, W_α = 0

At T_D: Only Solid (α) present

$W_{\mathcal{L}}$ = 0, W_α = 1.00



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Determination of phase weight fractions

- If there is only one phase, then the weight fraction of either solid or liquid will be 100 wt%,
- Example:

- Determine phase amount in the 2-phase Region:

  1- Draw the tie line.

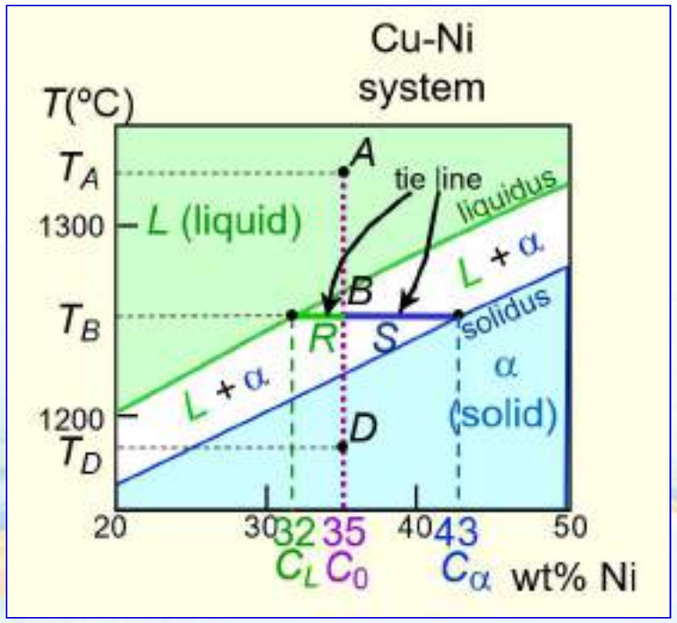
  2- Determine the distance from the point of interest (B) to each of the phase boundaries.

  $R = C_o - C_L$ and $S = C_\alpha - C_o$

  3- Mass fraction (wt%) of each phase:

$$W_L = \frac{S}{R+S} = \frac{C_\alpha - C_o}{C_\alpha - C_L} = \frac{43-35}{43-32} = 0.73$$

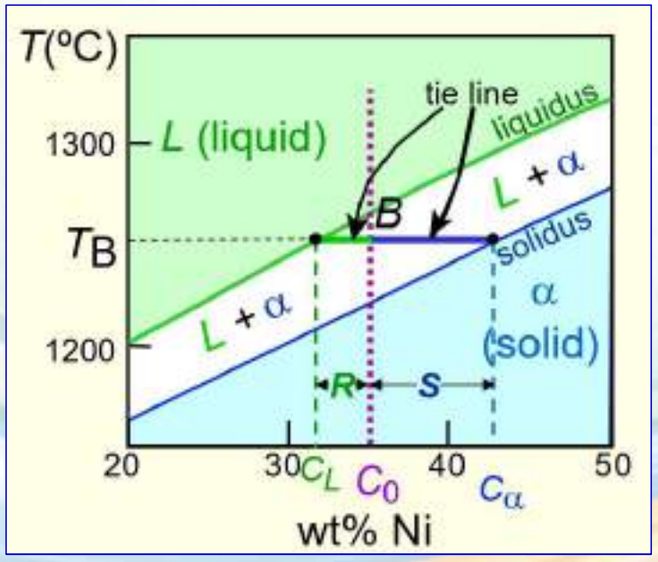
$$W_\alpha = \frac{S}{R+S} = \frac{C_o - C_L}{C_\alpha - C_L} = \frac{35-32}{43-32} = 0.27$$



i.e. 73% of the mass is liquid and 27% of the mass is solid.

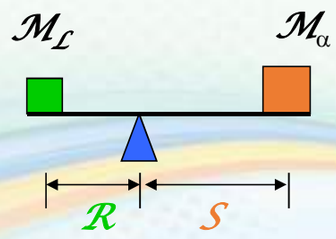
The Lever Rule

- *Tie line – connects the phases in equilibrium with each other – also sometimes called an isotherm*



What fraction of each phase?

Think of the tie line as a lever (teeter-totter)



$$M_\alpha \times S = M_L \times R$$

$$W_L = \frac{M_L}{M_L + M_\alpha} = \frac{S}{R+S} = \frac{C_\alpha - C_o}{C_\alpha - C_L}$$

$$W_\alpha = \frac{R}{R+S} = \frac{C_o - C_L}{C_\alpha - C_L}$$

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Development of microstructure in isomorphous alloys

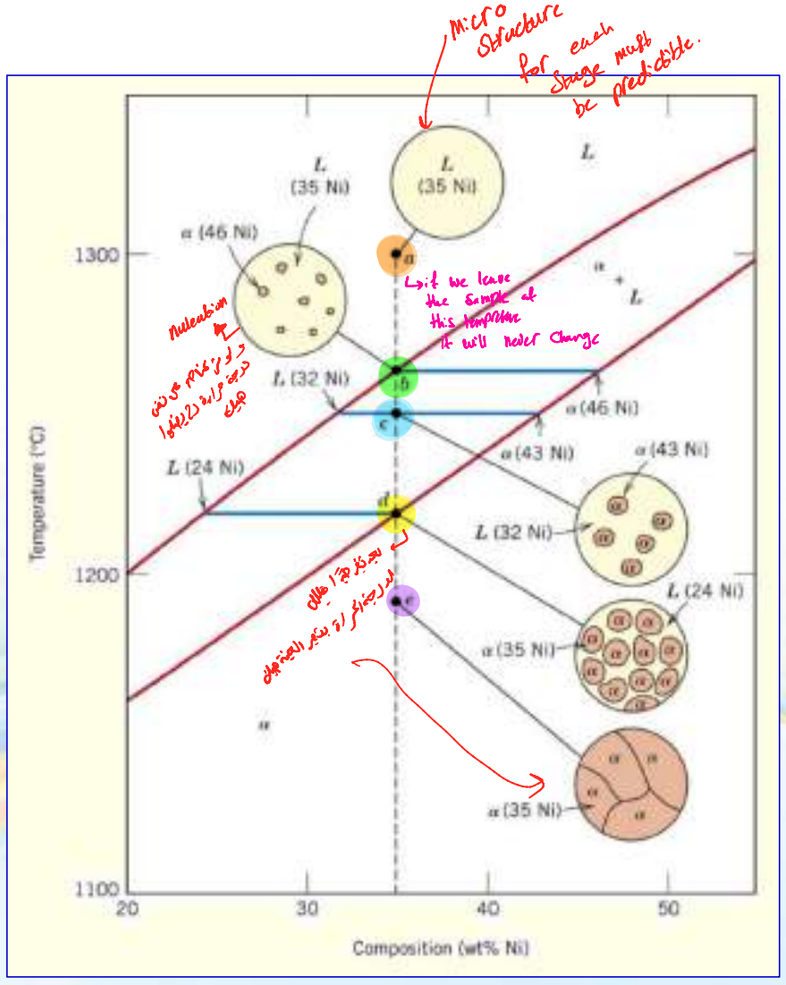
Equilibrium (very slow) cooling

- *Solidification in the solid + liquid phase occurs gradually upon cooling from the liquidus line.*
- *The composition of the solid and the liquid change gradually during cooling (as can be determined by the tie-line method).*
- *Nuclei of the solid phase form and they grow to consume all the liquid at the solidus line.*



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- *A (T>1300 °C): start as homogeneous liquid solution.*
- *B (T ~ 1260 °C): liquidus line reached. α phase begins to nucleate. C_α= 46 wt% Ni; C_L = 35 wt% Ni*
- *C (T= 1250 °C): calculate composition and mass fraction of each phase.*
- *D (T~ 1220 °C): solidus line reached. Nearly complete solidification. C_α= 35 wt% Ni; C_L = 24 wt% Ni*
- *E (T<1220 °C): homogeneous solid solution with 35 wt% Ni.*



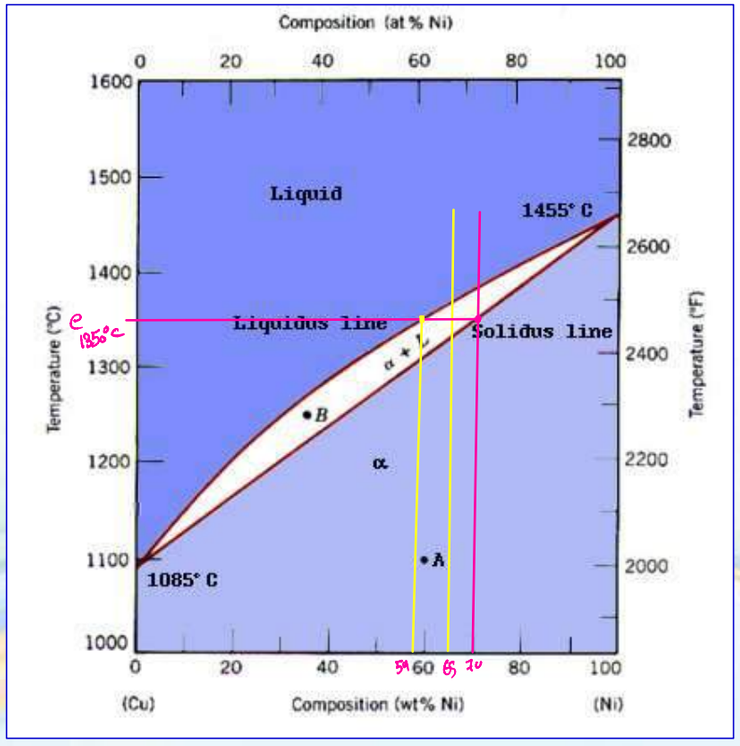
Example problem

65 wt% Ni – 35 wt% Cu alloy is heated to T within the α+L region. α-phase contains 70 wt% Ni, determine:

A) Temperature of the alloy.
B) Composition of the liquid phase.
C) Mass fraction of both phases.
↳ by Lever rule

$$L = \frac{70 - 65}{70 - 50}$$

$$V = (1 - L)$$



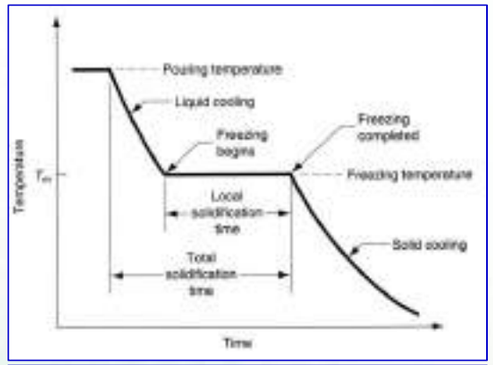
α = 70% of Nickel

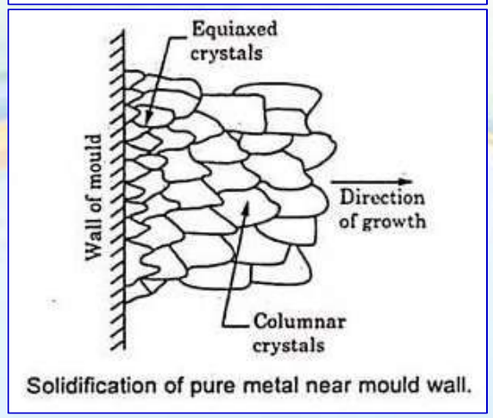
Development of microstructure in isomorphous alloys

- Non-equilibrium cooling
- Fast cooling, but how fast?

  → Fast w.r.t. diffusion. (diffusion: solid < liquid < gas)
- Since diffusion rate is especially low in solids, consider case where:
  - ✓ Cooling rate >> diffusion rate in solid
  - ✓ Cooling rate << diffusion rate in liquid

(equilibrium maintained in liquids phase)





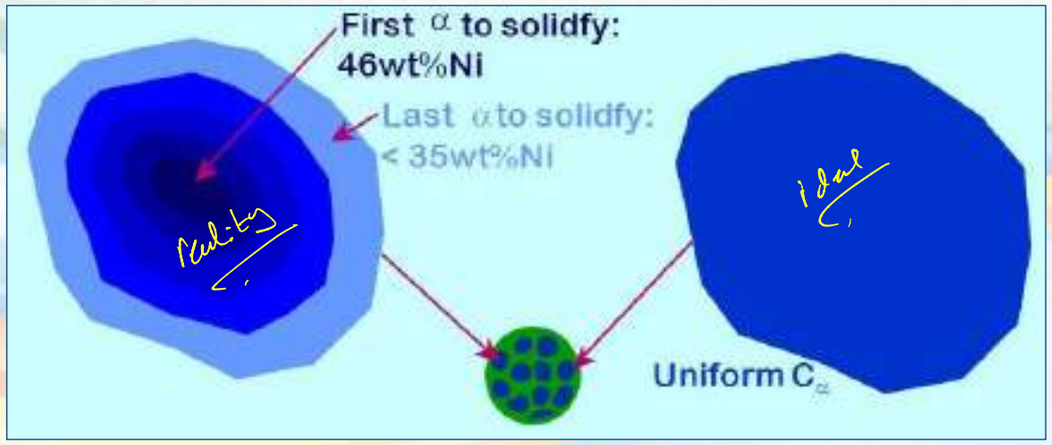
Solidification of pure metal near mould wall.

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Cored vs. Equilibrium Phases

- C_α changes Composition Upon Cooling
  - First α to solidify has C_α = 46 wt% Ni
  - Last α to solidify has C_α = 35 wt% Ni
- Fast Cool Rate — Slow Cool Rate

Cored structure — Equilibrium structure





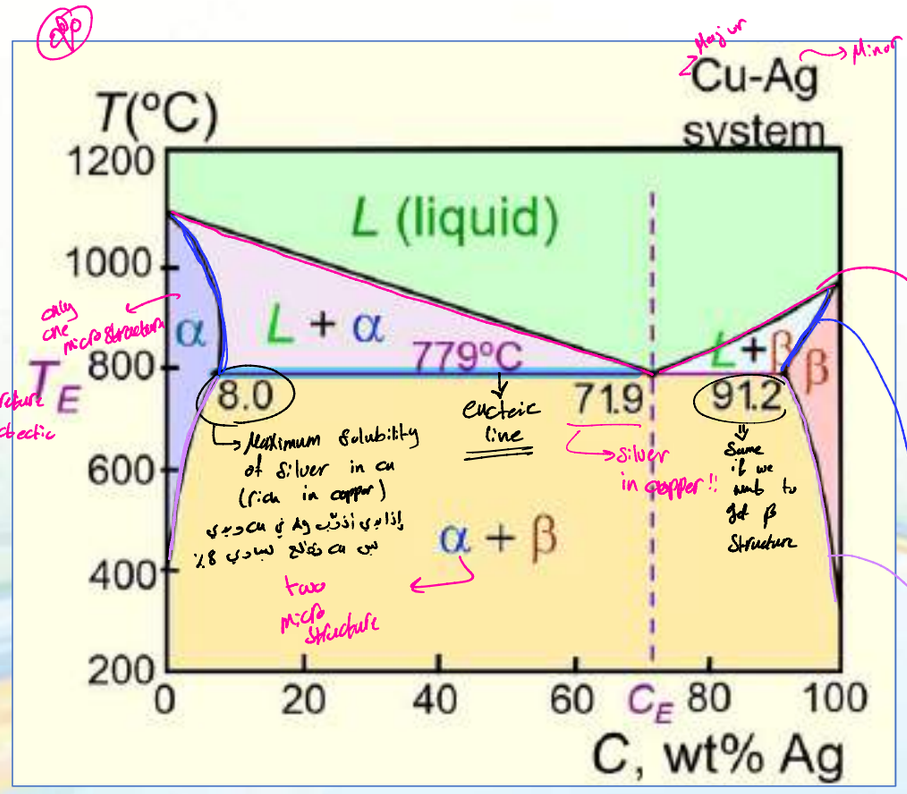
(α + β) => easily melted

⇒ remember
Lever rule apply only when the
Region had two or more phases
in one region at any temperature + composition.
in this diagram ⇒ (L + α) , (L + β) , (α + β)

عند زيادة درجة الحرارة عند نفس composition يحدث phase transformation

3- Binary Eutectic Systems ⇒ Second phase

- Binary: 2 components.
- Eutectic ⇒ "easily melted, has a special composition with a min. melting T". Sharp melting temperature @ composition ⇒ eutectic
- T_m (Cu = 1085 and Ag = 961.8 °C)



Liquidus line transform from Liquid → Liquid + β or α
↳ Liquid + Solid + Liquid (only)

Solidus line transform L+α → Solid α or L+β → Solid β
↳ Liquid + Solid + Solid (only)

Solvese line
↳ Solid + Solid
Solid → Solid transformation

عند هذا الخط لما أن L و α يكونان صحبة
لبعض أو تحولان كل الـ Liquid
وبتحوّل ← (β + α)

وعندنا α ← α & β
يلي كانوا بالـ (L + α)
و α بتزيد كمان من تحول (L)
ك (β + α) كمان!

Alpha eutectic

* β عند حين (L + β) عند تبقى

@ room temperature ⇒ only α, β only
α structure ⇒ range temperature

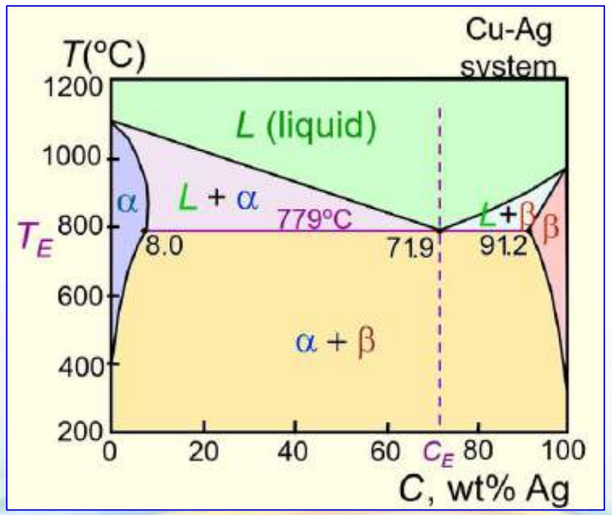
(α+β) ده long سؤال عشان كده عند ⊛ في السؤال
وطلع معنا β بـ 95 و α بـ 5

© = eutectic β الـ wt% كم ؟
eutectic line هي المستقيم الخط اللي أطلع من eutectic α الـ wt% كم ؟

95 من حاجة بالمية ← [Lever rule] α طلع

Binary Eutectic Systems

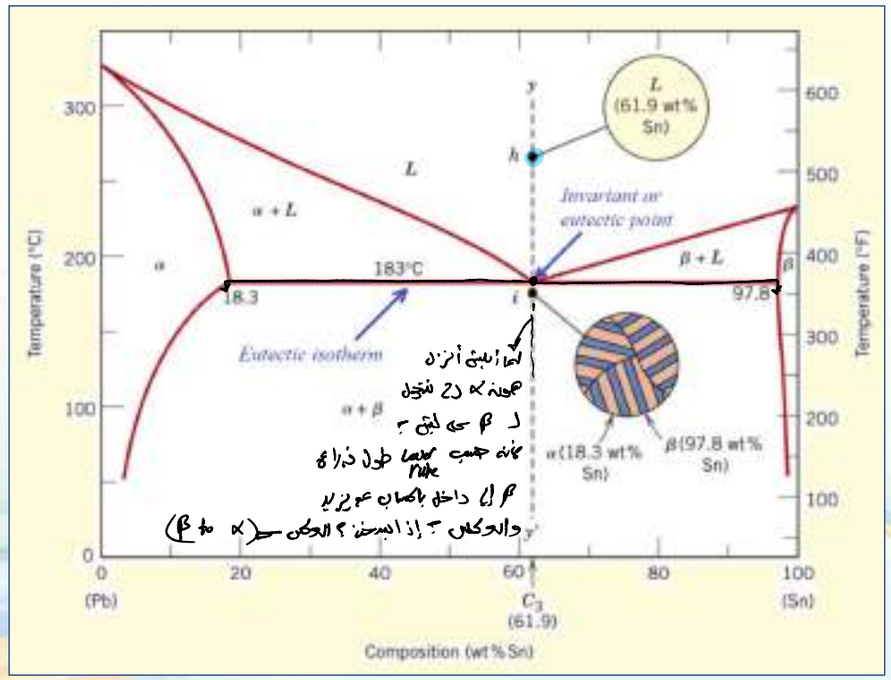
- **Single phase regions:**
  1. α-phase (solid solution rich in Cu).
  2. β-phase (solid solution rich in Ag).
  3. L-phase (liquid solution).
- **Phase coexistence regions:**
  1. α + β phases (limited solubility of Ag in Cu and vice versa lead to 2 different solid solution phases).
  2. α + L and β + L phase regions.



- Tie lines and Lever Rule can be applied in the 2-phase regions.
- Solvus line separates one solid solution from a mixture of solid solutions.

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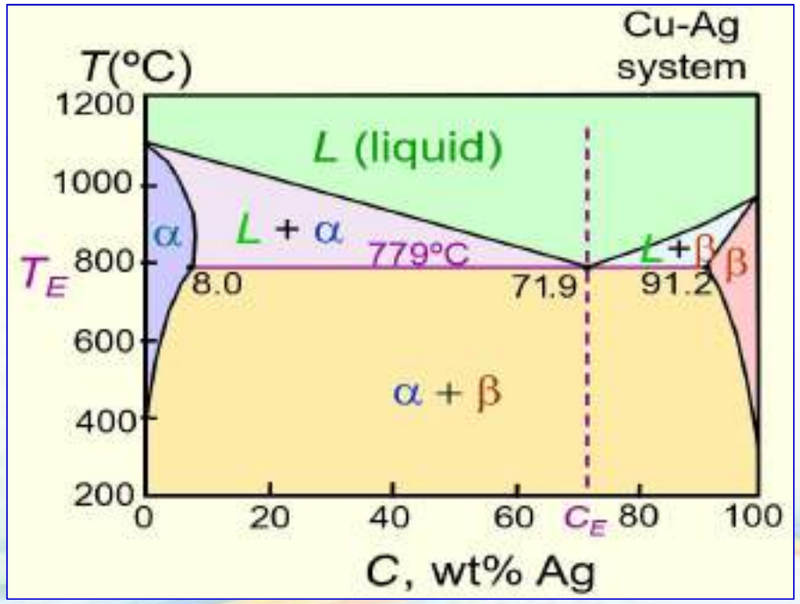
- *Eutectic or invariant point - Liquid and two solid phases co-exist in equilibrium at the eutectic composition C_E and the eutectic temperature T_E.*
- *Eutectic isotherm - the horizontal solidus line at T_E.*



183.1°C
↳ Liquid
182.9°C
↳ (α+β) Solid
Suddenly.

Ex.: Cu-Ag system

- *3 single phase regions ($\mathcal{L}$, α, β)*
- *Limited solubility:*
  α: *mostly Cu*
  β: *mostly Ag*
- T_E: *No liquid below* T_E
- C_E: *Composition at temperature* T_E
- *Eutectic reaction*
- $\mathcal{L}(C_E) \rightarrow \alpha(C_{\alpha E}) + \beta(C_{\beta E})$



$$L(71.9\ wt\%\ Ag) \leftrightarrow \alpha(8.0\ wt\%\ Ag) + \beta(91.2\ wt\%\ Ag)$$

Cooling ↓ ↑ *Heating*

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EX 1: Pb-Sn Eutectic System

- For a 40 wt% Sn-60 wt% Pb alloy at 150°C, determine:

1- The phases present

Answer: α + β

2- The phase compositions

Answer: C_α = 11 wt% Sn

C_β = 99 wt% Sn

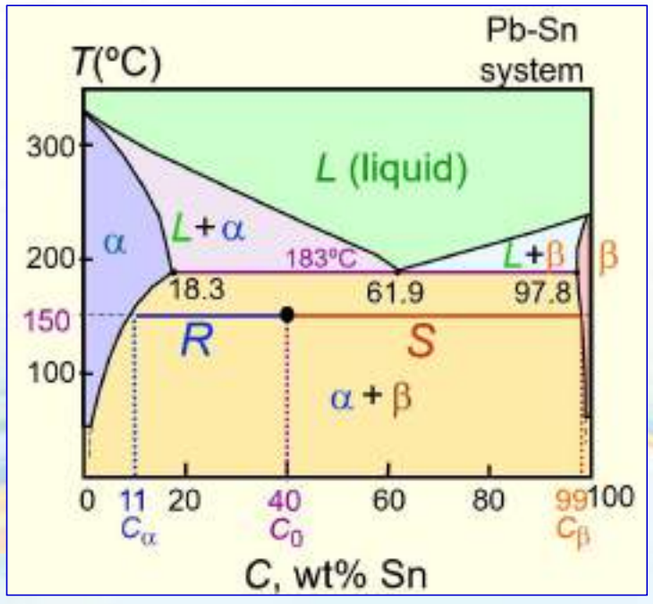
3- The relative amount of each phase

Answer:

$$W_\alpha = \frac{S}{R+S} = \frac{C_\beta - C_o}{C_\beta - C_\alpha} = \frac{99-40}{99-11} = \frac{59}{88} = 0.67 \hookrightarrow \frac{2}{3}$$

(مرفوض بالنظر)

$$W_\beta = \frac{R}{R+S} = \frac{C_o - C_\alpha}{C_\beta - C_\alpha} = \frac{40-11}{99-11} = \frac{29}{88} = 0.33 \hookrightarrow \frac{1}{3}$$



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EX 2: Pb-Sn Eutectic System

- For a 40 wt% Sn-60 wt% Pb alloy at 220°C, determine:

1- The phases present:

Answer: α + L

2- The phase compositions

Answer: C_α = 17 wt% Sn

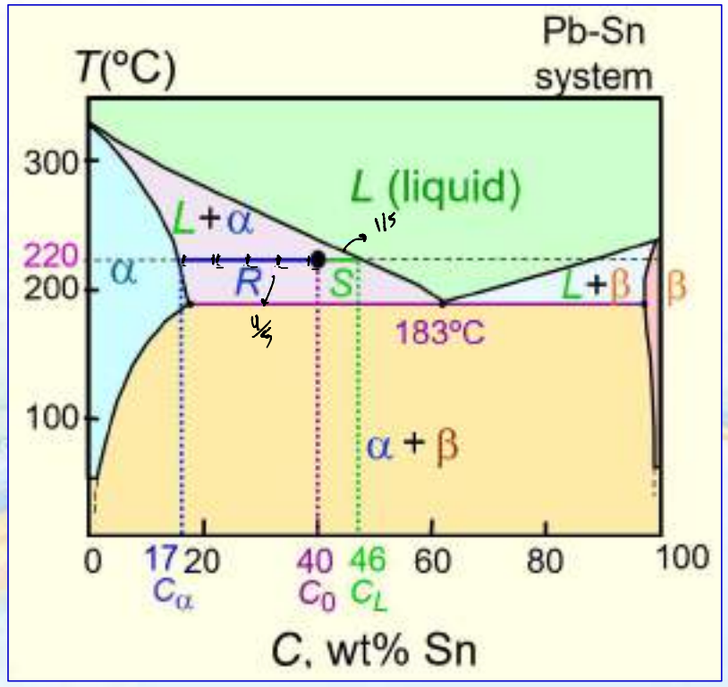
C_L = 46 wt% Sn

3- The relative amount of each phase

Answer:

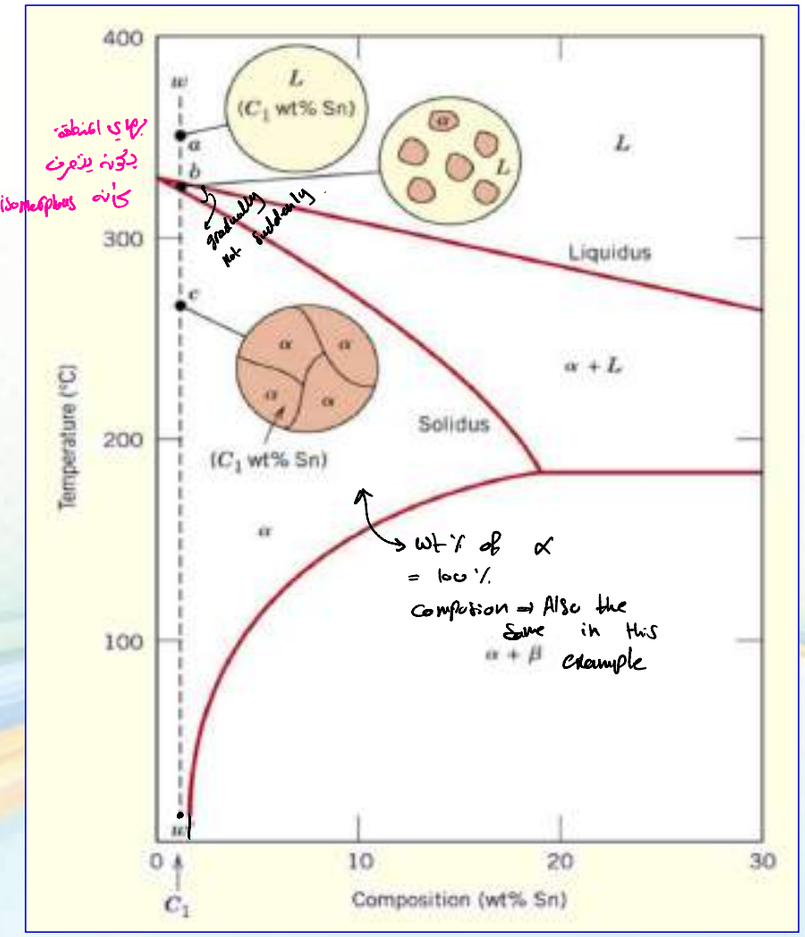
$$W_\alpha = \frac{C_L - C_o}{C_L - C_\alpha} = \frac{46 - 40}{46 - 17} = \frac{6}{29} = 0.21$$

$$W_L = \frac{C_o - C_\alpha}{C_L - C_\alpha} = \frac{23}{29} = 0.79$$



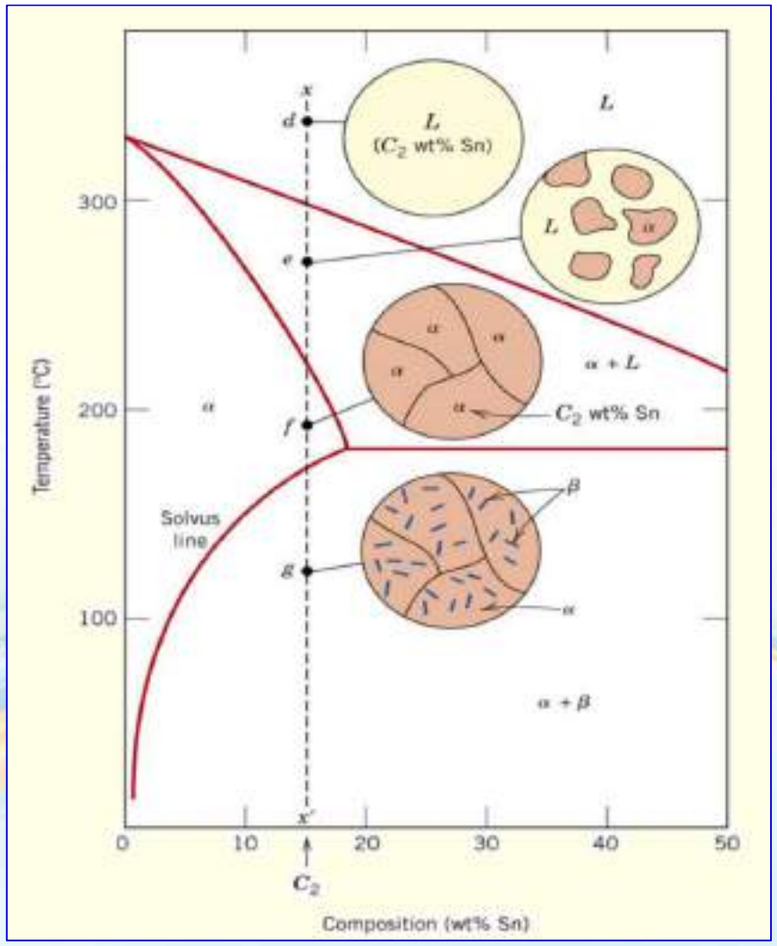
Microstructural Developments in Eutectic Systems I

- For alloys for which C_0 < 2 wt% Sn
- Result: at room temperature
  - ✓ Polycrystalline with grains of a phase having composition C_0



Microstructural Developments in Eutectic Systems II

- For alloys for which 2 wt% Sn < C_0 < 18.3 wt% Sn
- Result:
  - ✓ Initially liquid + α
  - ✓ Then α alone
  - ✓ Finally at temperatures in α + β range: Polycrystalline with α grains and small β-phase particles



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Chapter 8

Applications and Processing of Metal Alloys

The University of Jordan
Chemical Engineering Department

Spring 2022

Prof. Yousef Mubarak

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ISSUES TO ADDRESS...

→ General classification
ferrous and nonferrous.

- How are metal alloys classified and what are their common applications?
- What are some of the common fabrication techniques for metals?
- What heat treatment procedures are used to improve the mechanical properties of both ferrous and nonferrous alloys? (will not be covered this semester)



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Classification of Metal Alloys

Metal Alloys ⇒ based on the main constituent of the metal.

Contains iron ↩

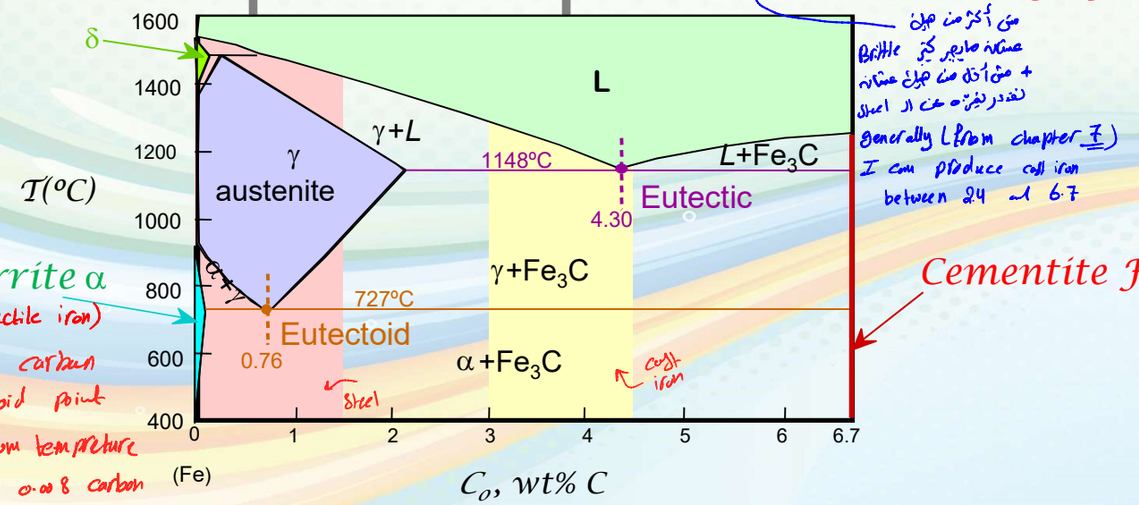
Ferrous

Nonferrous

Steels
<1.4wt% C

Cast Irons ← recommended amount of carbon.
3-4.5 wt% C

microstructure: ferrite, graphite/cementite



Ferrite α
(ductile iron)
0.022 of carbon of eutectoid point but of room temperature it contains 0.008 carbon

Cementite Fe3C

Brittle حتى أكثر من هذا مسامية مايبقى كتير + صعب أكثر من هذا مسامية تتقدر تغيرها على الـ steel
Generally (from chapter 7) I can produce cast iron between 2.4 and 6.7

Yousef Mubarak

Materials Science

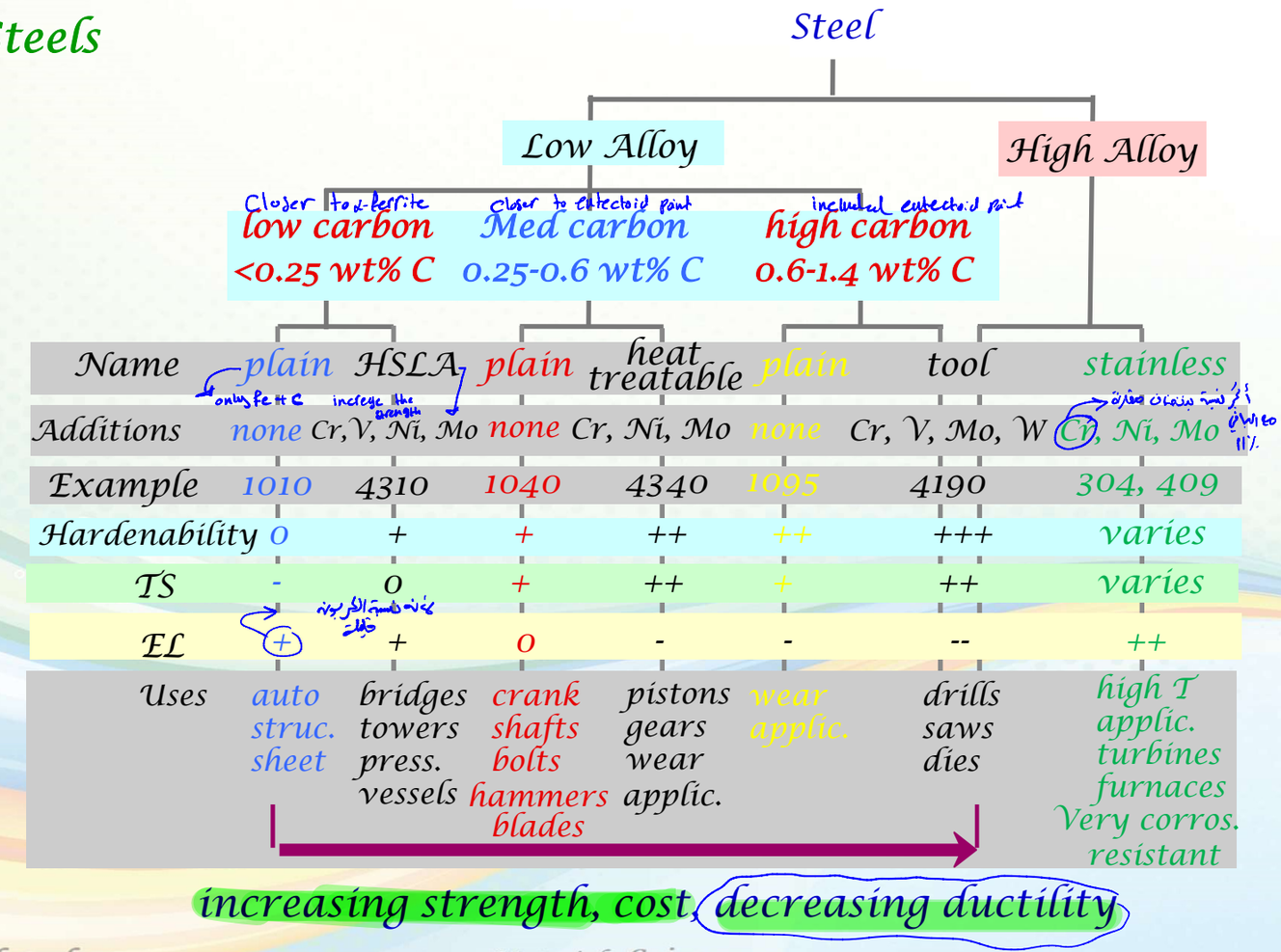
increasing of concentration of cementite

The reflection of the brittleness of steel and cast iron is how much there is cementite in it (as the concentration of cementite ↑, the brittleness ↑)

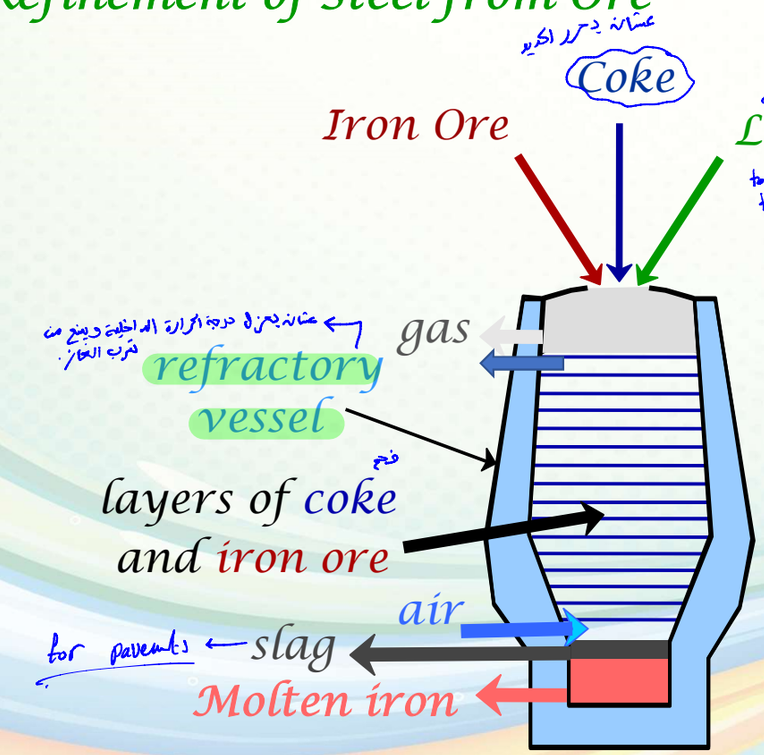
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lo ⇒ only carbon at Fe

Steels



Refinement of Steel from Ore



heat generation

$$C + O_2 \rightarrow CO_2$$

reduction of iron ore to metal

$$CO_2 + C \rightarrow 2CO$$

$$3CO + Fe_2O_3 \rightarrow 2Fe + 3CO_2$$

purification

$$CaCO_3 \rightarrow CaO + CO_2$$

$$CaO + SiO_2 + Al_2O_3 \rightarrow slag$$

Ferrous Alloys

- Iron-based alloys:
  - Steel
  - Cast Irons
- Nomenclature for steels (AISI/SAE)

10xx	Plain Carbon Steels
11xx	Plain Carbon Steels (resulfurized for machinability)
15xx	Mn (1.00 - 1.65%)
40xx	Mo (0.20 ~ 0.30%)
43xx	Ni (1.65 - 2.00%), Cr (0.40 - 0.90%), Mo (0.20 - 0.30%)
44xx	Mo (0.5%)

where xx is wt% C x 100

Example: 1060 steel – plain carbon steel with 0.60 wt% C

Stainless Steel >11% Cr

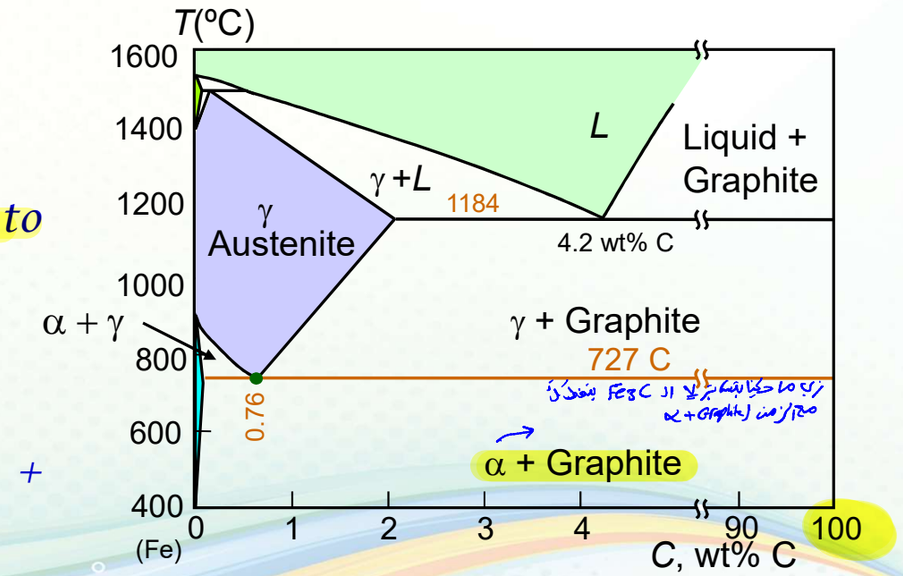
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Cast Irons

- Ferrous alloys with > 2.1 wt% C
  - More commonly 3 - 4.5 wt% C
- Low melting – relatively easy to cast ⇒
- Generally brittle
- Cementite decomposes to ferrite + graphite

$Fe_3C \rightarrow 3\,Fe\,(\alpha) + C\,(graphite)$

- This decomposition process is generally a slow process



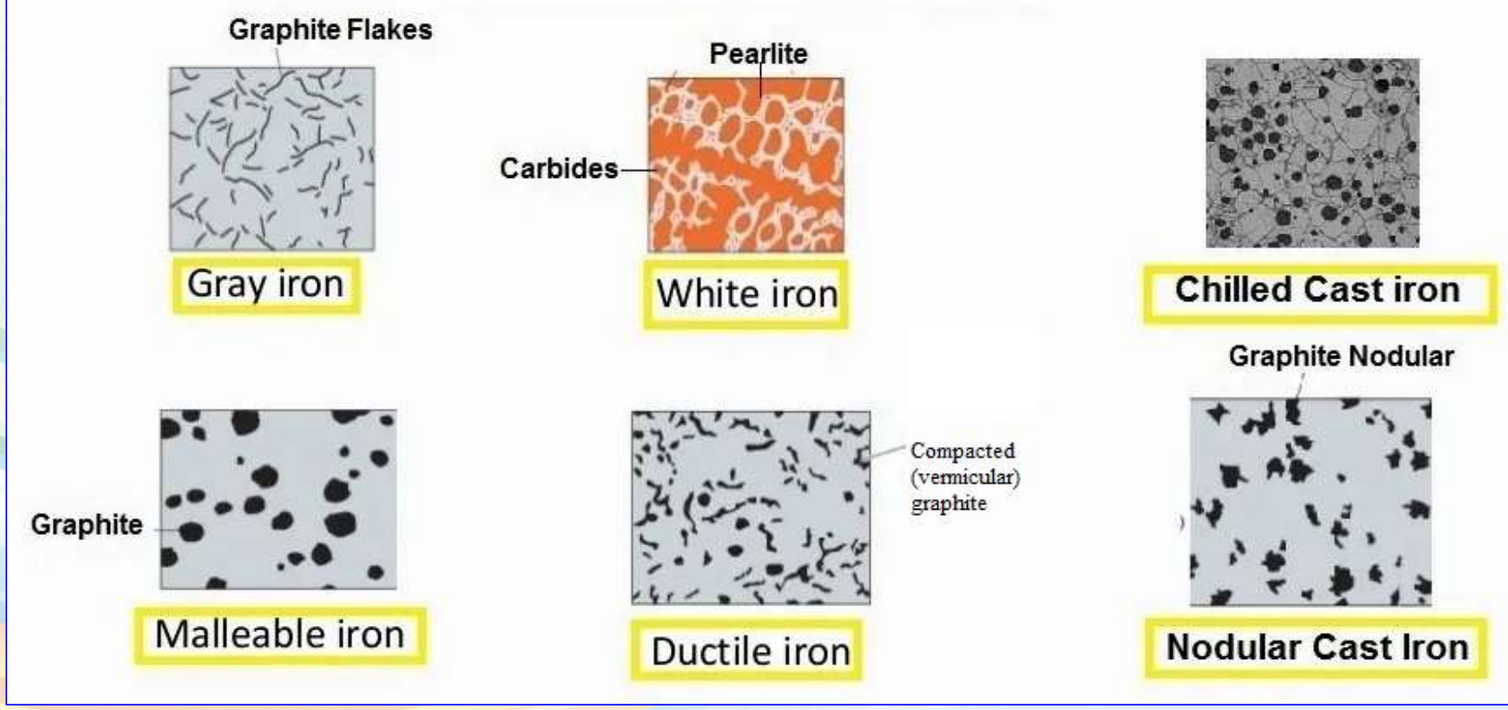
Graphite formation promoted by:

- ✓ Si > 1 wt%
- ✓ slow cooling

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Types of Cast Iron

↳ Based on the additives + the technique



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Types of Cast Iron

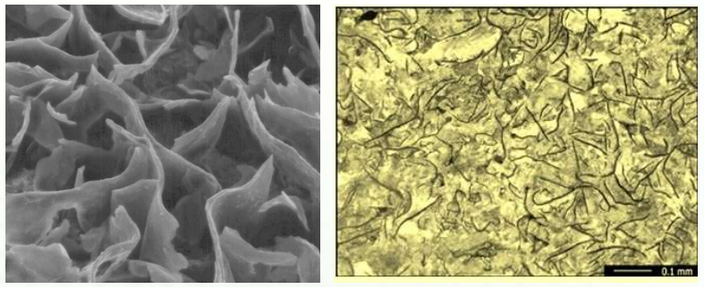


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Types of Cast Iron

Gray Iron

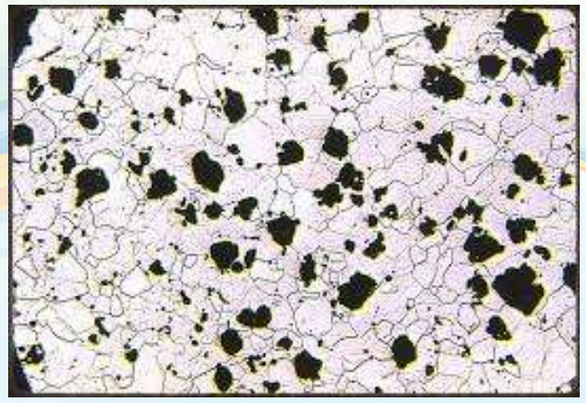
- Graphite flakes
- Weak & brittle in tension
- Stronger in compression ← يستخدم لهذا الغرض
- Excellent vibrational dampening (مثال)
- Wear resistant



Ductile Iron

- Add Mg and/or Ce
- Graphite as nodules not flakes
- Matrix often pearlite – stronger but less ductile

ferrite + cementite.

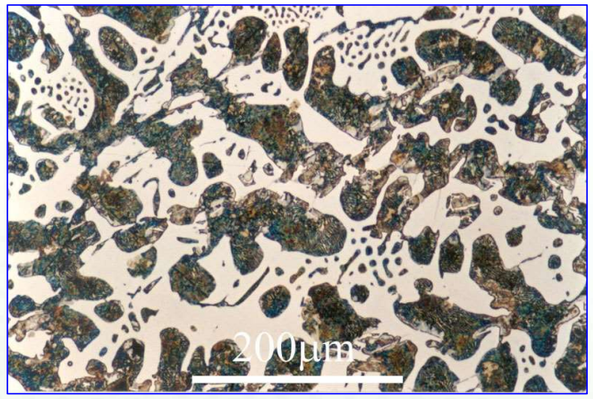


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Types of Cast Iron

White iron → Nat. Combin graphite

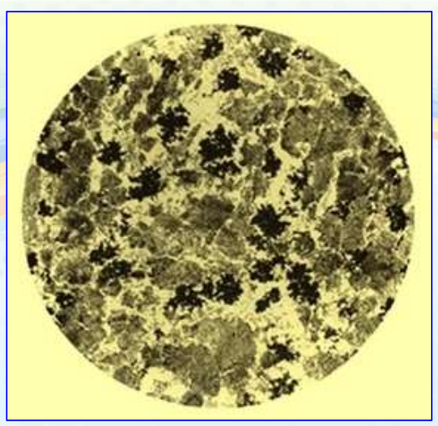
- < 1 wt% Si
- Pearlite + cementite
- Very hard and brittle



Malleable iron

→ for several hours

- Heat treat white iron at 800-900°C
- Graphite in rosettes ⇒ decomposed of cementite in the oven.
- Reasonably strong and ductile
  → because it contains now graphite

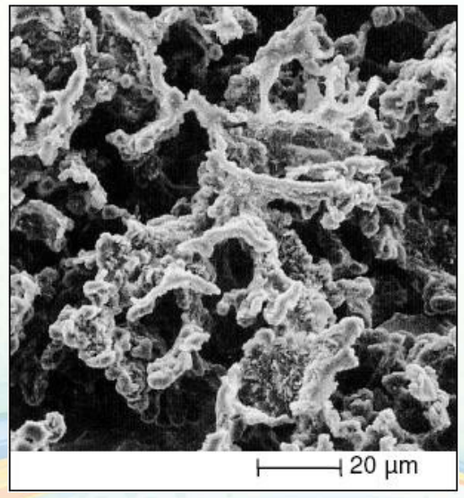


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Types of Cast Iron

Compacted graphite iron

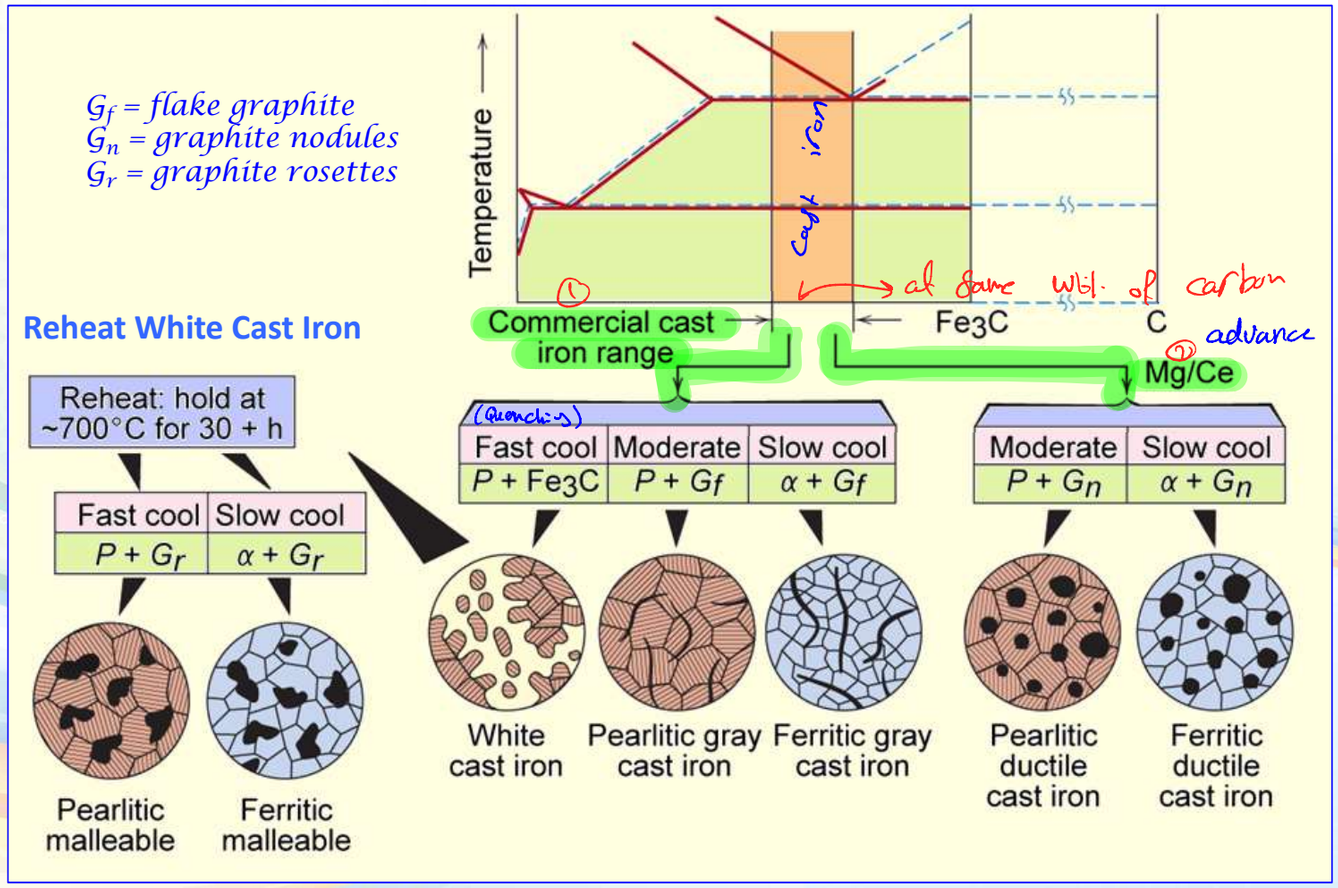
- Can be prepared by addition of small amount of Ce or Mg to gray cast iron
- Relatively high thermal conductivity
- Good resistance to thermal shock
- Lower oxidation at elevated temperatures



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Production of Cast Irons

G_f = flake graphite
G_n = graphite nodules
G_r = graphite rosettes



① at same Wt. % of carbon
② advance cast iron Mg/Ce

P => pearlite
Gn => Graphite as nodules
Gf => Graphite as flakes
GR => Graphite as rosebs.

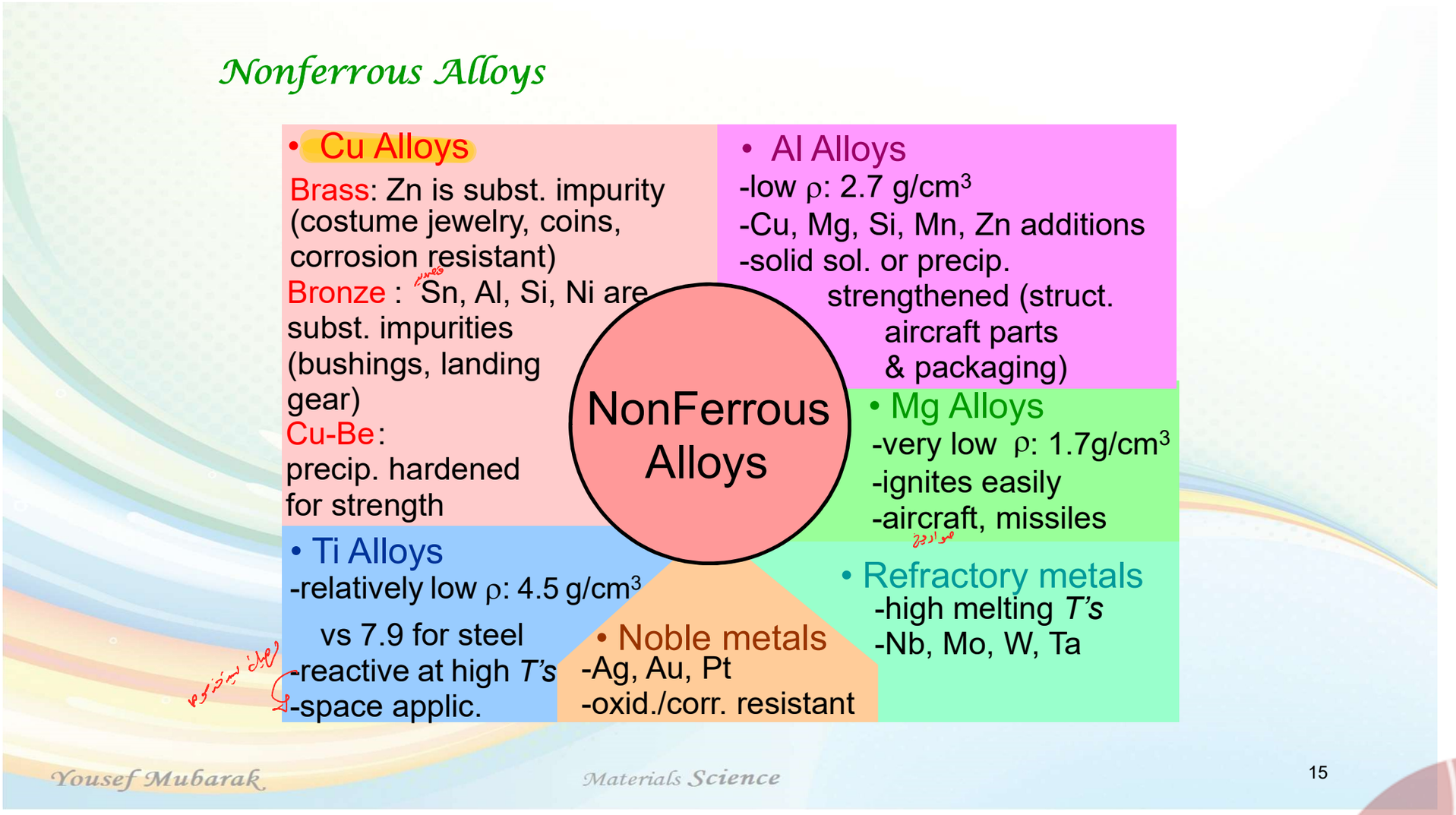
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Limitations of Ferrous Alloys

- One main drawback of ferrous alloys is their environmental degradation i.e. poor corrosion resistance.
- Other disadvantages include:
  1) Relatively high densities.
  2) Relatively low electrical conductivities
  3) High cost to finish product
- In ferrous materials the main alloying element is carbon

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Nonferrous Alloys



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Metal Fabrication

- How do we fabricate metals?
  - Blacksmith - hammer (forged)
  - Cast molten metal into mold
- Forming Operations
  - Rough stock formed to final shape

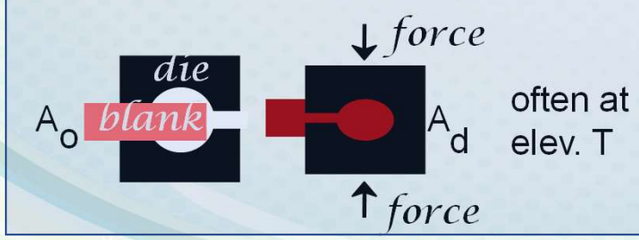
Hot working	vs.	Cold working
✓ Deformation temperature high enough for recrystallization		✓ Deformation below recrystallization temperature
✓ Large deformations		✓ Strain hardening occurs
		✓ Small deformations

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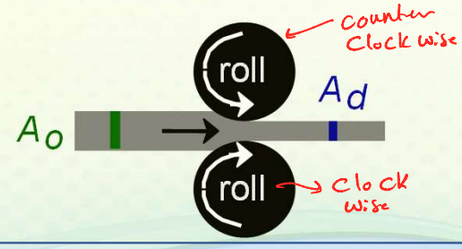
Metal Fabrication Methods (i)

FORMING | CASTING | JOINING

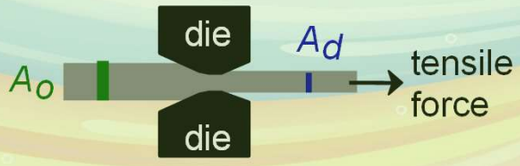
Forging (Hammering; Stamping)
(wrenches, crankshafts)



Rolling (Hot or Cold Rolling)
(I-beams, rails, sheet & plate)

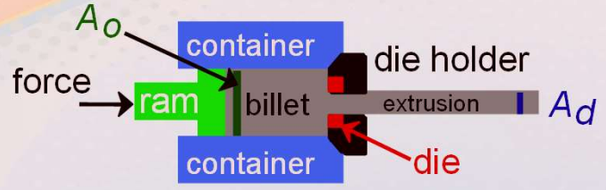


Drawing
(rods, wire, tubing)



die must be well lubricated & clean

Extrusion ⇒ for metals at high T.
(rods, tubing)



ductile metals, e.g. Cu, Al (hot)

forging:

بنحبب قطعة من المادة وبرفع درجة حرارتها عشانة تمر الـ Soft بحرية بدخلها على قالب التشكيل (die) ويكبس عليها بـ force صحيحة وجالس بخليها تشكل زي بدّي إيا بالضبط.

drawing:

applied force بالاتجاه عكس الاتجاه اللي بال rolling أول ما بدأ ال force بتكون بالاتجاه اللي بدي إياه (die) بحيث يكون فيها ضغوط شد وبحبب بسحبها باستخدام قوة الشد.

Rolling:

بنحبب ال billet وهيه بتمر مع عشرين اشي rollers والثانية الحكي عشانة يقلل عندي Thickness Thickness بتبعت هاي المادة ، بقدر أتحكم بال Thickness بدّي بدي إياه عن طريق زيادة أو نقصانة بال rollers بدّي بيت هدول ال rollers إذا كانت صعب أسحبها Hot working => ductile Cold working => ductile

Extrusion:

بنحبب المادة اللي بدنا نشكلها (Billet) بترفع درجة حرارتها لـ (elev T) بحيث بحطوها بال container بحيث بحطوا ال die اللي بدّي يحتوي على شكل اللي بدي إياه ثم بحبب الـ billet وبطلع شكل الناتج.

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Metal Fabrication Methods (ii)



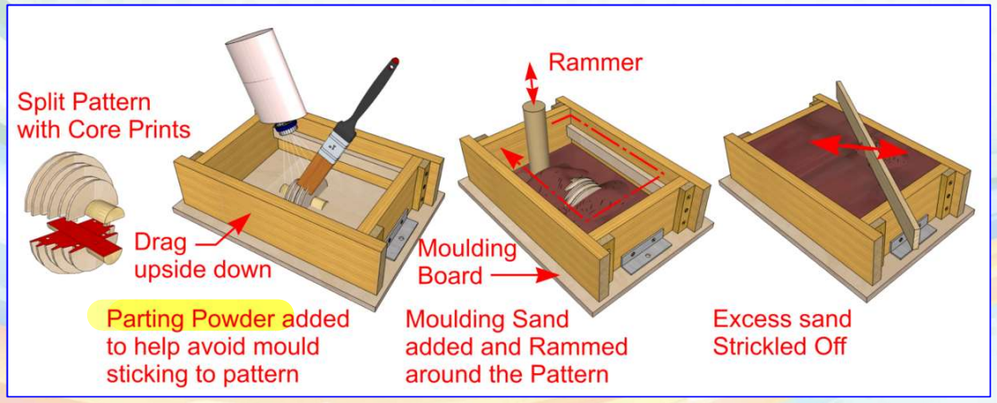
- Casting- mold is filled with molten metal
  - Metal melted in furnace, perhaps alloying elements added, then cast in a mold
  - Common and inexpensive
  - Gives good production of shapes
  - Weaker products, internal defects
  - Good option for brittle materials

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Metal Fabrication Methods (ii)

FORMING | **CASTING** | JOINING

- **Sand Casting**
  (large parts, e.g., auto engine blocks)



- What material will withstand $T > 1600°C$ and is inexpensive and easy to mold?

  Answer: sand!!!

- To create mold, pack sand around form (pattern) of desired shape

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Metal Fabrication Methods (ii)

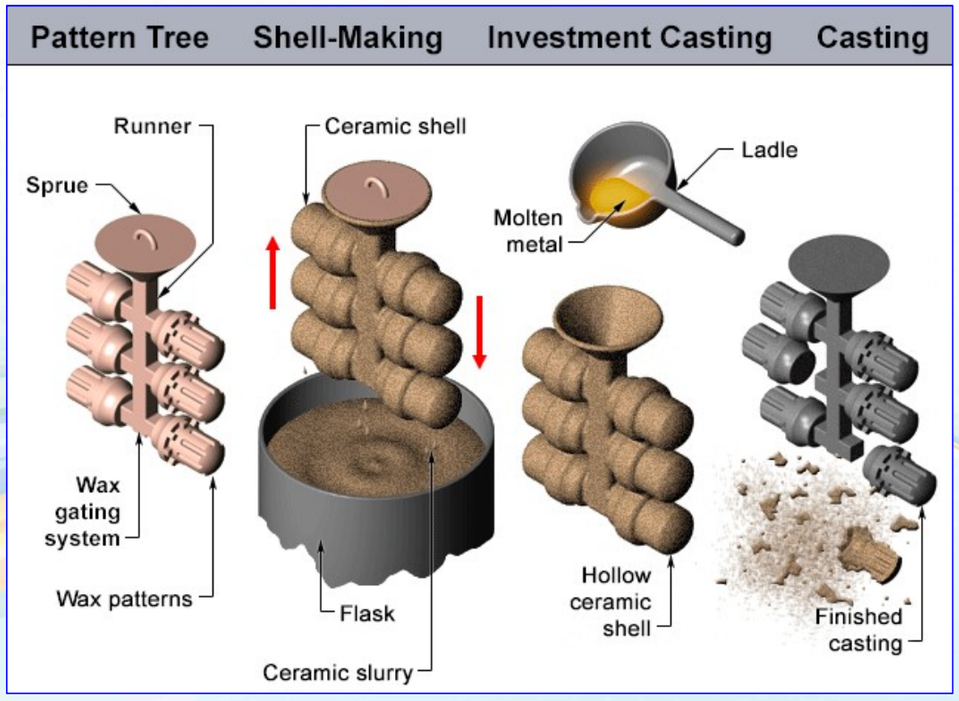
FORMING | CASTING | JOINING

- ***Investment Casting*** *(low volume, complex shapes e.g., jewelry, turbine blades)* ⇒ for one more than one item.

Stage I: Mold formed by pouring plaster of paris around wax pattern. Plaster allowed to harden.

Stage II: Wax is melted and then poured from mold—hollow mold cavity remains. ⇒ الخلية صغيرة لحد ما يوصل سمك 1-4 inch wall

Stage III: Molten metal is poured into mold and allowed to solidify.



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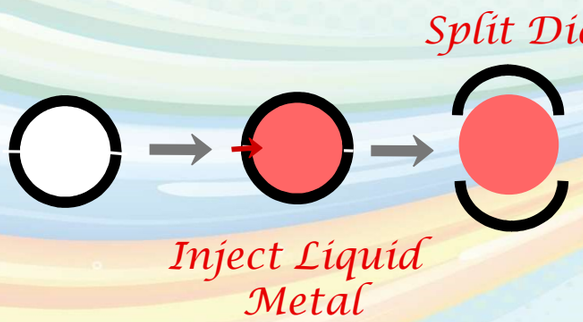


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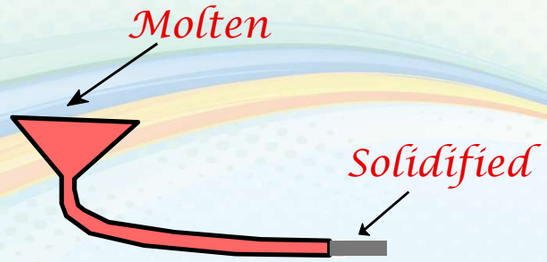
Metal Fabrication Methods (ii)

FORMING | **CASTING** | JOINING

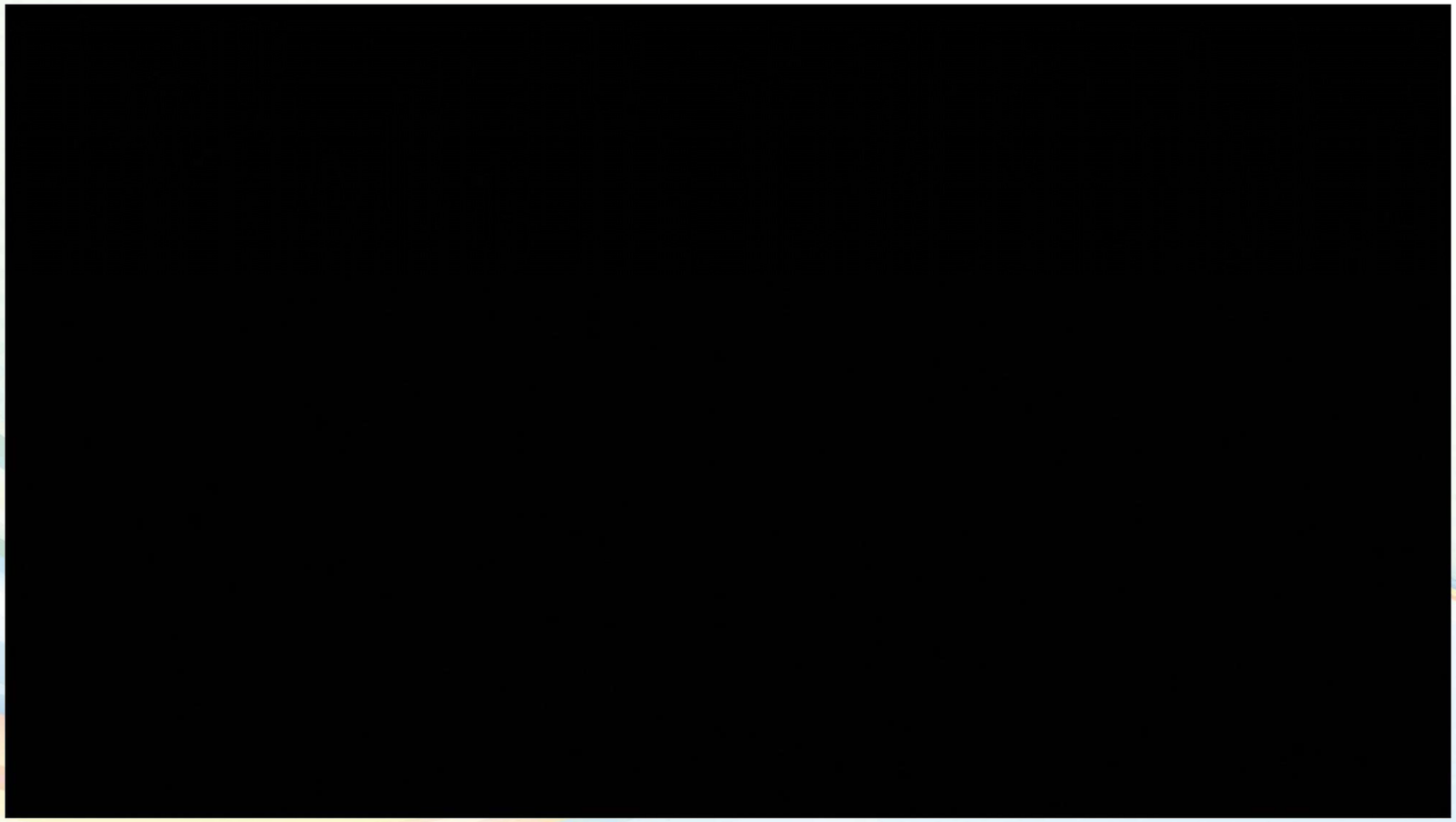
- **Die Casting** → not for hollow products
  - High volume
  - For alloys having low melting temperatures



- **Continuous Casting**
  - Simple shapes: rectangular slabs, cylinders

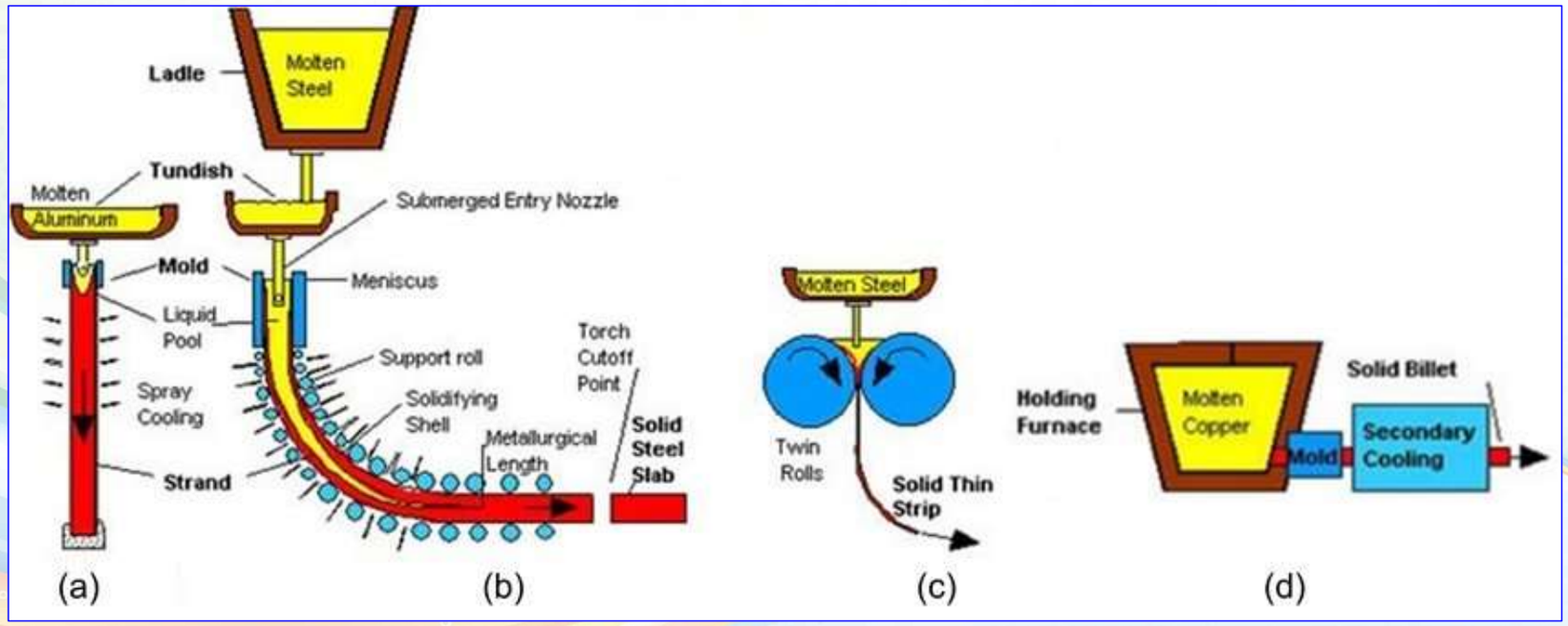


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Continuous Casting

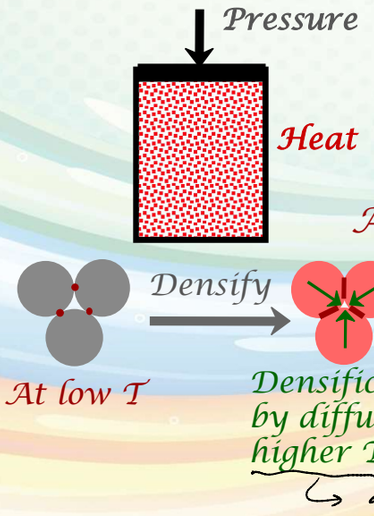


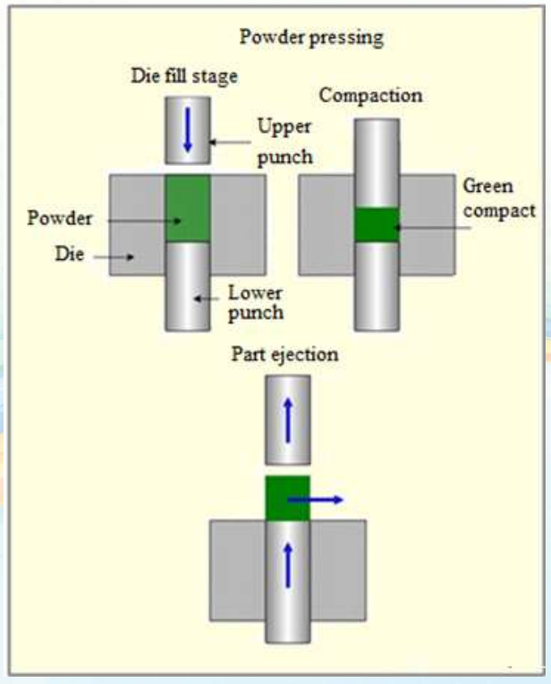
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Metal Fabrication Methods (ii)

FORMING | CASTING | **JOINING**

- **Powder Metallurgy**
  (metals with low ductility)





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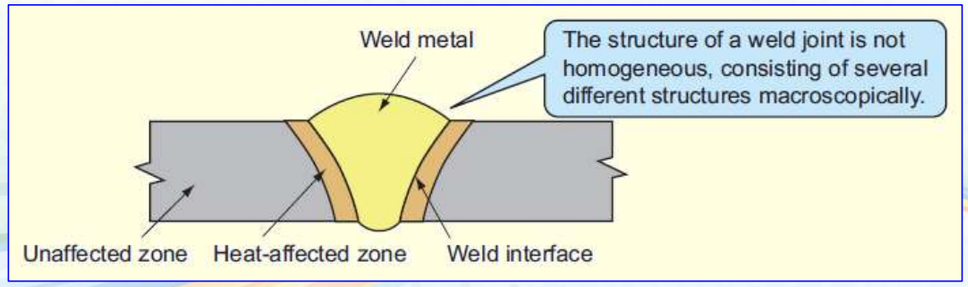
Metal Fabrication Methods (ii)

FORMING | CASTING | JOINING

- **Welding** → rolling then welding good for producing large tanks.

  (when fabrication of one large part is impractical)

- *Heat-affected zone: (region in which the microstructure has been changed).*



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