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Continuous change

دفتر :

علم مواد

Material Science

First

للطالب : عبدارحمن تيّم

اللجنة الأكاديمية لقسم الهندسة الصناعية

2023

Smart Material:

① Pictoelectric Material

② Piezo Magnatic Material

③ electro Magnatic Material

Magno electric Material

the same

④ Pyro electric Material

Introduction

- Historical perspective:
  - Materials found everywhere around us and effects the quality of our life.
  - The development and advancement of societies are tied to their members ability to produce and manipulate material to fit their needs.

- Materials drive our society
  - **Stone Age**
  - **Bronze Age**
  - **Iron Age**
  - **Now?**
    - Silicon Age? ⟶ Electronic components and semiconductors
    - Polymer Age? ⟶ Biotechnology and Energy applications
    - Smart materials and Nano-materials Age ⟶ Electronics

Designation is based on the level of material development

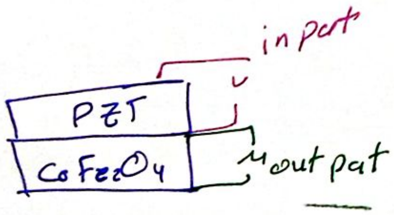
Si, Ge → Semi أشهر مادة

أطراف صناعية

ألواح شمسية

تكلفة تصنيع قليلة

③ electro Magnatic

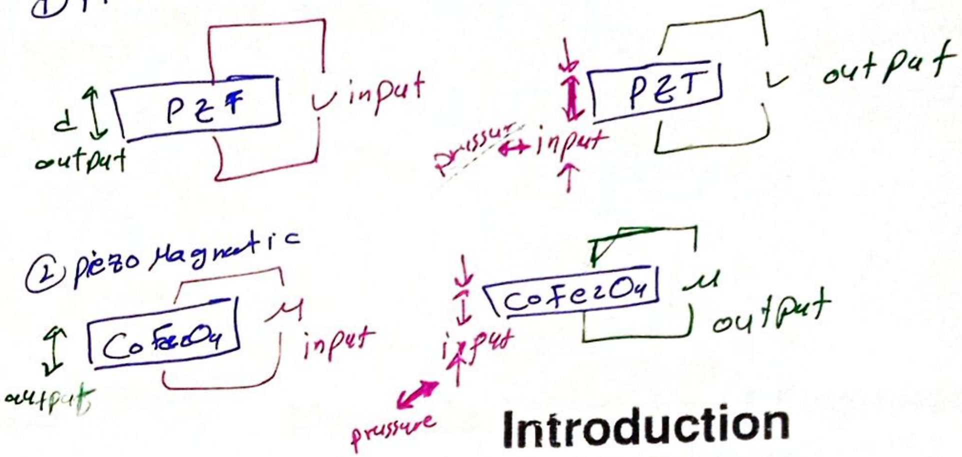


الجيرمانيوم أفضل من السيليكون ولكنه غالي ونادر ← يستخدم السيليكون

← السيليكون يستخدم كثيراً في Barrels

① Piezoelectric

② piezo Magnatic



PZT:-
أفضل نوع piezoelectric لأنه بأقل ضغط جهد بـ تمدد عالي

CoFe2O4
أفضل نوع piezo Magnatic لأنه بأقل ضغط مجال بـ تمدد عالي

Introduction

- **Naturally occur materials**: stone, skin, bone, wood.
- **Synthetic materials:** discover techniques (heat treatment, and addition of other substances) to produce materials that have superior properties to the natural ones, i.e. metals.
- **Advanced materials:** knowledge acquired over approximately the past 100 years after understanding relationship between material structure and its properties.

~~Polymer Age:~~

* أي مادة تحتوي بوليمر رحما من استخدامها مدوليا بنسبة معينة لا تصدم

* الرحما عن بحاي الـ sesitivity عالي ← مفيد في الـ sensors

Why do we study materials science and engineering?

- Many engineers will at one time or another exposed to a design problem involving materials. Properties of materials; Cost and availability; Performance; Processing technique.
- Examples
  - Mechanical Engineer: Transmission gear design.
  - Chemical Engineer: Oil refinery component.
  - Electrical Engineer: Integrated circuit chip.
  - Civil Engineer: Superstructure of building.
  - Industrial Engineer: Design of ....?

Materials Science and Engineering

Related with Atoms {inside structur}

- What is material science? Materials science is a fundamental science concerned with the relationship between the structure and properties of materials. [Fundamental science (or basic science, pure science) ... fundamentals and knowledge.]
- What is material engineering? Materials Engineering takes those materials and applies them to real world problems, by knowing the properties of a particular material engineers design or fabricate that material for desired applications. [Applied science: the application of scientific knowledge transferred into real-world problems.]

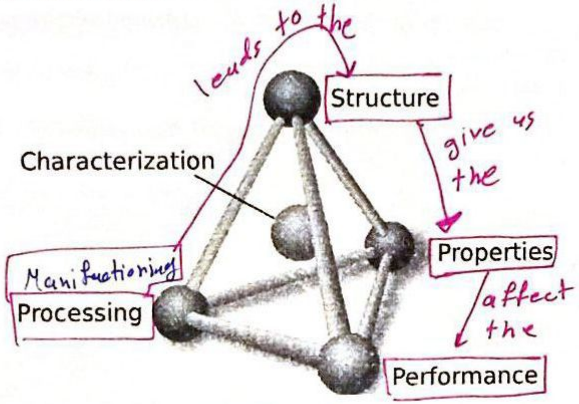
use the properties in Applied field

- What are the basic components of the materials science and engineering? (material tetrahedral)

- 3 different process leads to 3 different structures
- Al_2O_3 {appears like powder}

Materials Science and Engineering Elements

1) Structure
2) Properties
3) Processing
4) Performance



Materials Tetrahedron

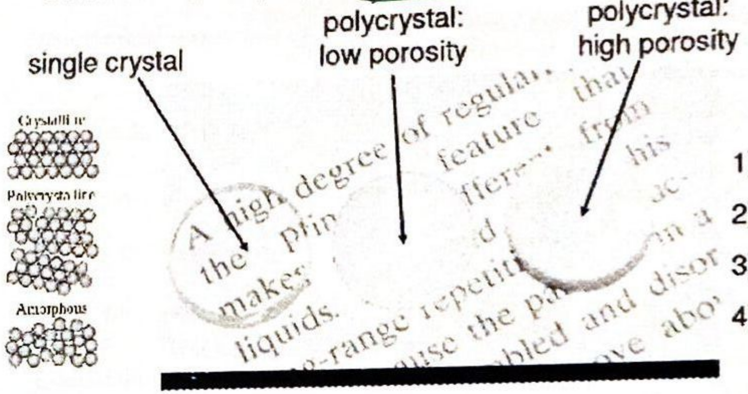
→ every single element we have to test it {characterizaition}

→ Characterizaitoio of structre {telescope}
→ " " properties {run carreft}

OPTICAL

important

- Transmittance: Aluminum oxide {Al_2O_3} may be transparent, translucent, or opaque depending on the material structure.



1) Structure
2) Properties
3) Processing
4) Performanc e

Polycrystalline materials are solids that are composed of many crystallites of varying size and orientation.

Adapted from Fig. 1.2, *Callister 7e.* (Specimen preparation, P.A. Lessing; photo by S. Tanner.)

The structre control the propertics of the material rather than anything else

Material Property

- Definition: it is the material attribute in terms of kind and magnitude of response to a specific imposed stimulus. → {need, external effiction to test}
- The properties of solid materials can be grouped into different categories:
  - Mechanical
  - Electrical
  - Thermal
  - Magnetic
  - Optical
  - Deteriorative: The act or process of becoming worse.
  - Material property is independent of its size and shape.

- powder processing {technology}

compared with casting

⊕
- Tempreture
- time
- aquercy
- safety
- semifinished
- control the structure
- القالب ثابت

⊖
- cost
- ~~size of the object~~

⊕ - size of obj

{- large material can't use the powder processing}

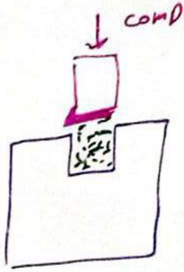
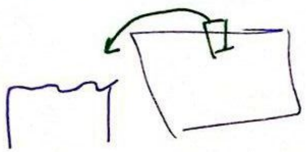


Table 1 Material properties and qualities

Properties	Qualities
Physical properties	Density, melting point, damping capacity
Mechanical properties	Yield, tensile, compressive and torsional strengths, ductility, fatigue strength → cyclying load test, constront load test ← creep strength, fracture toughness
Manufacturing properties	Ability to be shaped by molding, casting, plastic deformation, powder processing, machining. Ability to be joined by adhesives, welding, and other process
Chemical properties	Resistance to oxidation, corrosion, solvents, and environmental factors
Other non-mechanical properties	Electrical, magnetic, optical and thermal properties
Economic properties	Raw material and processing cost. Availability
Aesthetic properties	Appearance, texture and ability to accept special finishes

* Requaiured recognizing type of properties

→ Surface Roughness {to test the Aesthetic properties}



$R_a = \square\ \mu m$

- calculate the area under the curve
- (Ra) less → خشونة أقل

{Ra value should be [4–10] μm}

used to Advanced cases

SEM TEM

{needs Advance Machiens to study}

for chemical Analysis study

Material Structure

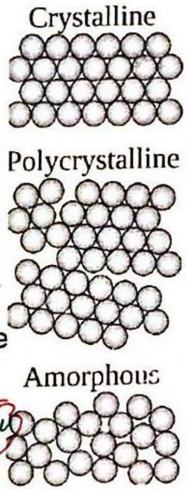
Definition: Arrangement of its internal component.

Bottom-up study approach:

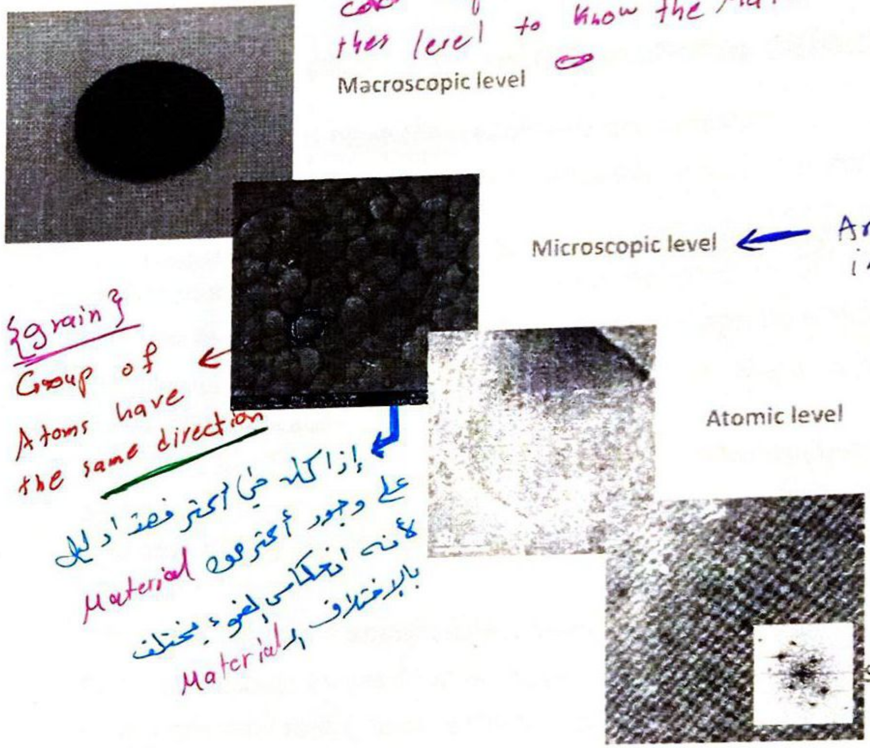
- **Subatomic level:** involves electrons within individual atoms and interactions with their nuclei. $\{10^{-10}\,m\}$ TEM
- **Atomic level:** encompasses the organization of atoms or molecules relative to one another. $\{10^{-9}-10^{-8}\}$ SEM
- **Microscopic level:** contains large group of atoms that are normally agglomerated together. (Microscopic means it can be observed by some type of microscope). $\{10^{-6}\}$ SEM
- **Macroscopic level:** involves the structural elements that may be viewed with the naked eye. $\{10^{-3}\}$ {seen with base eyes}

naked eye

for Material Analysis study



color important in this level to know the Material contained

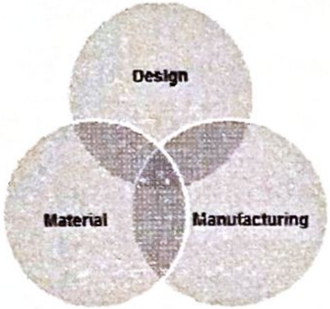


Area of itrest in this course

{grain}
Group of Atoms have the same direction

إزاكله جي أكتر فضة ادليل
على وجود أكترمن Material
لأنه انعكاس الضوء مختلف
بالإختلاف الـMaterial

Design, materials and manufacture?



nterrelationships: **Design** problem involving materials...selecting the right **naterials...manufacturing** processes

The more familiar an engineer with the various characteristics and structure-roperties relationship, and processing techniques; the more proficient and onfident she/he will be to make good choices based on the selection criteria's."

Points to be consider upon material selection?

- **Does the material have the necessary properties?**

  Ex. Strength and ductility...range of materials suitable for the job
  In-service conditions...stability.
  Ex. Reduction in mechanical strength / high temperature / corrosive environments)
- **Can the material be formed to the desired design and shape?**

  Manufacturability; ...manufacturing process. Processing techniques...will effect the properties
- **Will the material be adversely affected by environmental conditions and environmental interaction?** Will the properties of the material alter with time during service? Will the material resist corrosion and other form of attack?
- **Will the material be acceptable on aesthetic grounds?**
- **Can the product be made at an acceptable cost?**
- **Environmental and social factors...**Safe

→ Sintering: treatment to raise the toghness for the Material. {Heat treatment}
it happenes under high temprutre {ceramic}

→ Annealing: treatment to raise the ductitity {Heat treatment}

The Materials Selection Process

1. Application ⟶ Determine required Properties
   Properties: mechanical, electrical, thermal, magnetic, optical, deteriorative.
2. Properties ⟶ Identify candidate Material(s)
   Material: structure, composition.
3. Material ⟶ Identify required Processing
   Processing: changes *structure* and overall *shape*
   ex: casting, sintering, vapor deposition, doping
   forming, joining, annealing.

→ Vapor deposition: {electronics}
treatment that used to made voltage difference on non-electronic Material

→ Forming: Changing the shape of the material {metals} by pruser

→ joining: Ataching two things to each ather

→ Doping: Adding a particular Material to Another

Classification of materials*

- Metals
- Ceramics
- Polymers

} Main classes of materials

- Composites → componisition between two materials or more
- Semiconductors si
- Biomaterials Te
- Nanomaterials ← material in nano level
- Smart materials

} Advanced materials

Mentioned prevically

* Classification criterion: chemical make up and atomic structure

Composit → recognized with naked eyes
→ the spacers seen
- in room tem
- separated propenities still as it is

Alloy → can't see a seperated materials
→ the spacers non-seen
- required liquid case
- High tem

→ New properities

* The Metals is crestilized

→ All the atoms neatly appears

Metals*

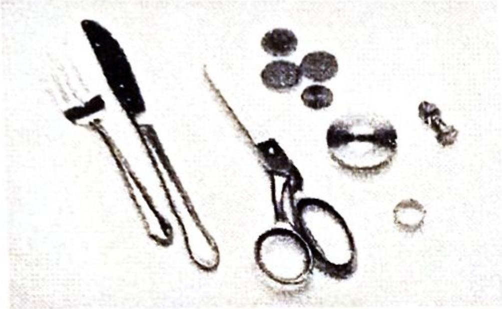
Composed of one or more metallic elements, and often nonmetallic element in a relatively small amount.

Structure:

Atoms arranged in a very orderly manner. Relatively dense. Large number of non-localized electrons.

Properties: → Tensile

Strong, Stiff, ductile. High thermal & electrical conductivity. Opaque, reflective.



Application examples

The term metal alloy is used to refer to a metallic substance that is composed of two or more elements.

---

* Ceramic :- input material → powder

* Automizition

عملية صناعة البودرة بالتحويل

من سائل إلى صلب ← ع شكل حبيبات

* يستخدم من الأغراض لأنه يتحمل درجة حرارة عالية

Transisto & diods made of ceramic

①+②+③ {Main components for ceramics}

Ceramics *

* Compounds between metallic and nonmetallic elements.

Common ceramics: ① Oxides, ② carbides, ③ nitrides, clay minerals (porcelain), cement, and glass.

Properties: ثانوي → Compression

Strong, stiff, very hard, brittle. Insulator (low electrical conductivity). Resistance to high temperature and harsh environments. Optical behavior: transparent, translucent, or opaque.

Application examples

* The final step of Manifacturing the ceramics most likely is Polishing

* Atomization :-

*من يعملوها بنحط بودرة في قالب و بنضغطه

Polymers

Organic compounds that are chemically based on C, H, and other nonmetallic element (O, N, Si).

Structure:

Large molecular structure chain-like in nature, have backbone of C atoms

Properties:

Low density. Non strong, not stiff (strength/mass is good), ductile, and pliable. Inert chemically and unreactive. Tend to soft/decompose at high temperatures. Low conductivity, nonmagnetic.

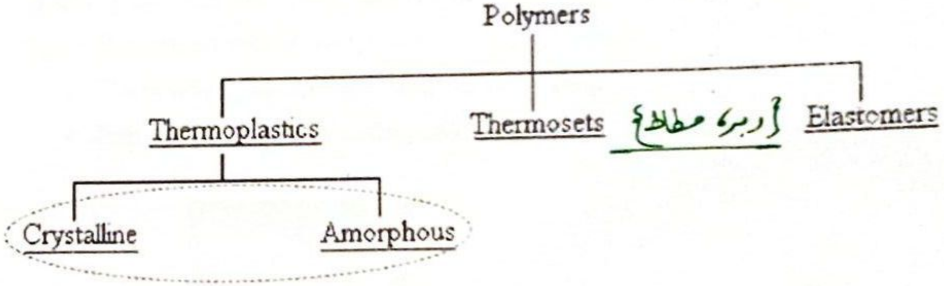
Application examples

ultra violet {light}

important factor of manifacturing the polymers

→ نفس فائدة الناموس

Classification of Polymers



- Polymers
  - Thermoplastics
    - Crystalline
    - Amorphous
  - Thermosets {ربرة مطاط}
  - Elastomers

Later…Ch:5

* Recycable *

- **Thermoplastic (TP)** – Polymers that can be shaped when heated and regain original hardness & strength upon cooling, in other words, a polymer that becomes pliable or moldable above a specific temperature, and returns to it's original solid state upon cooling.
  - Have a linear or branched structure.
  - Most thermoplastics have a high molecular weight, whose chains associate through intermolecular forces; this property allows thermoplastics to be remolded because the intermolecular interactions spontaneously reform upon cooling.
  - Process is reversible. cycle Manifacturing is easy in these kind of Material
  - Example: Cellulosics, nylons, polyethylenes, polyvinyl chloride...etc

non-recyclable

- **Thermoset (TS)** – is polymer material that irreversibly cures.

  Have a three-dimensional networked (strong secondary bonds), in which there is a high degree of cross-linking between polymer chains. The cross-linking restricts the motion of the chains and leads to a rigid material.
  - Process is irreversible.
  - Thermosets cannot be reshaped by heating.
  - Example: Epoxy, polyester, urethane, phenolics, silicones

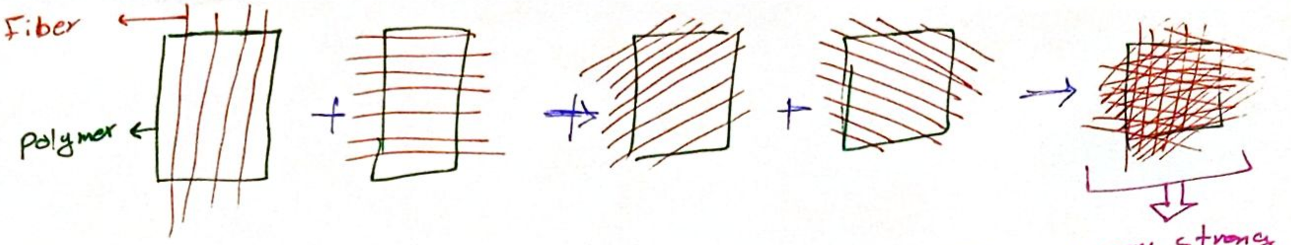
** **

Curing is a term in polymer chemistry and process engineering that refers to the toughening or hardening of a polymer material by cross-linking of polymer chains, brought about by chemical additives, ultraviolet radiation, electron beam or heat. In rubber, the curing process is also called vulcanization

مطاط ⇒ ما بتعيد تصنيعه ولك
بتتلفها

Thermoplastic && Thermoset

Read about 3D-Print



we aim to raise the ratio $\frac{strength}{mass}$

→ very strong Material can carry an Axial load in most directions in 3D Plane

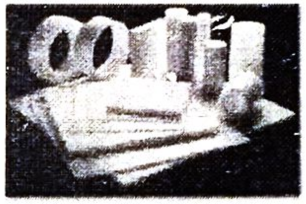
Elastomer (Rubber) –are rubbery polymers that can be stretched easily to several times their un-stretched length and which rapidly return to their original dimensions when the applied stress is released.

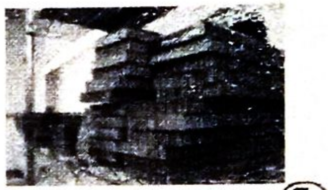
Elastomers are cross-linked, but have a low cross-link density. The polymer chains still have some freedom to move, but are prevented from permanently moving relative to each other by the cross-links.

Tires, foot wear, gaskets,..

Composites

- Combination of more than one material it could be naturally-occurring or synthetic (man-made).
- Designed to display (incorporate) a combination of the best characteristics (properties) of each one of the component materials.
- Example: Fiber glass embedded within a polymeric material.
  - Fiber glass: strong and stiff (but also brittle)
  - Polymer: ductile , low density (but also weak and flexible)
  - Composite: stiff, strong, flexible, and ductile. { collecting properties }
- Example: Polyte-tra-flouro-ethylene (PTFE) is a composite material of polymer and metal, used as bearing material.

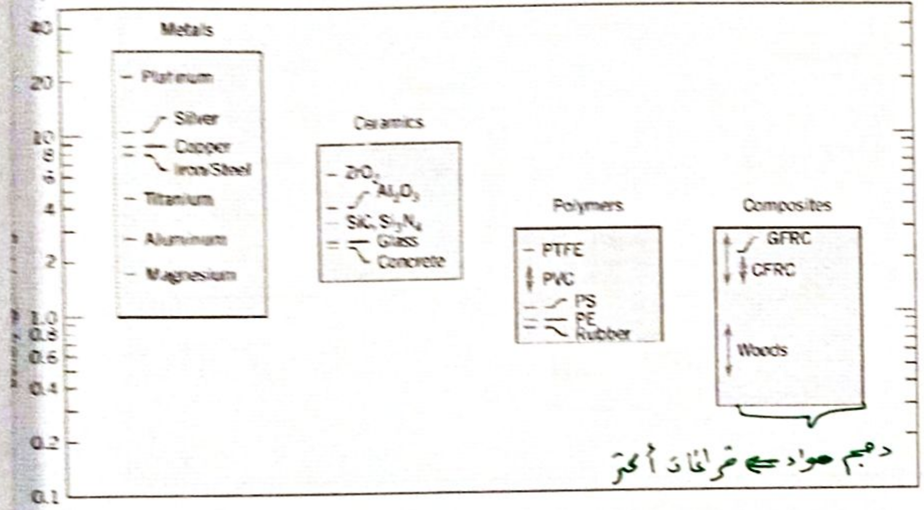




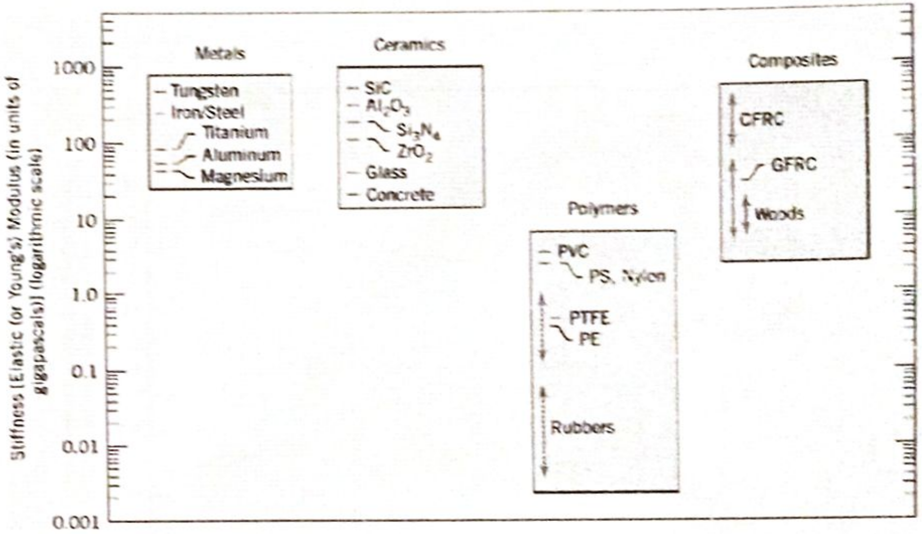
PTFE →

important to Manifacturue Bearings with low mass than Metals

→ Density



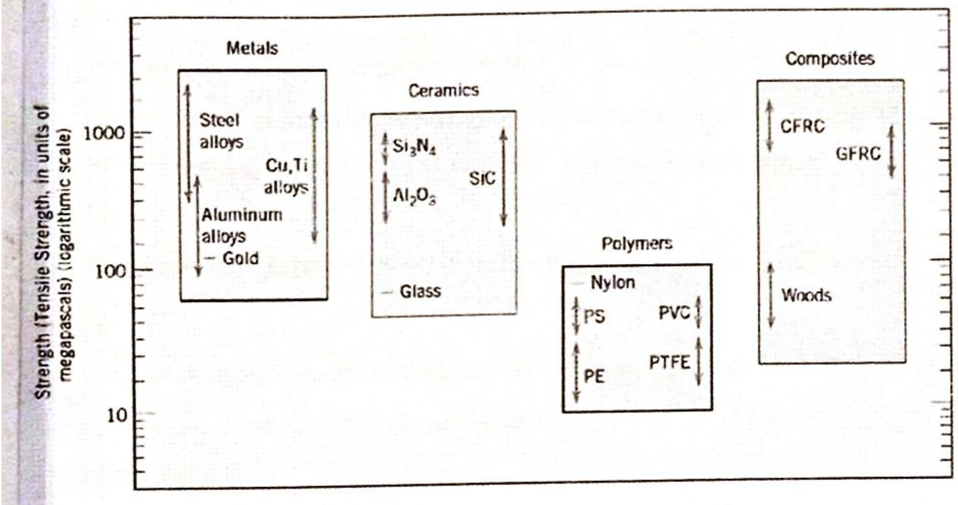
دمج مواد ⟸ فراغات أكثر

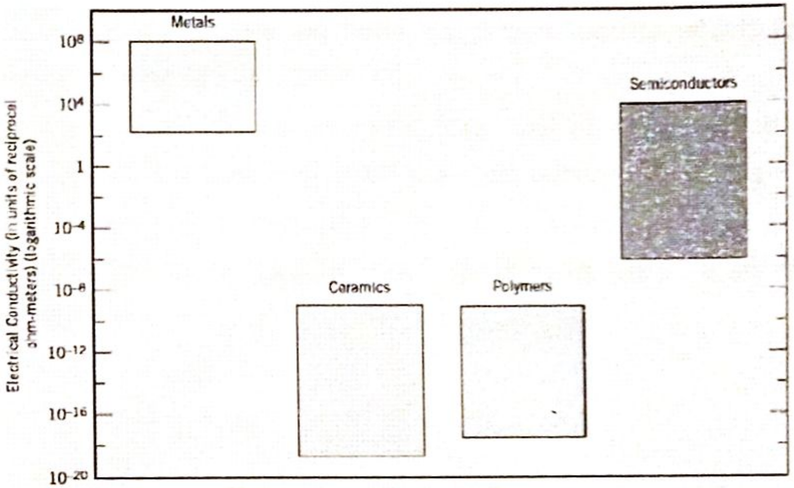


→ Mercury Density Measurment

→ used to find the non-uniform shapes Value

بتعبئة زئبق


Strength (Tensile Strength, in units of megapascals) (logarithmic scale)
1000
100
10
Metals
Steel alloys
Cu,Ti alloys
Aluminum alloys
Gold
Ceramics
Si_3N_4
Al_2O_3
SiC
Glass
Polymers
Nylon
PS
PVC
PE
PTFE
Composites
CFRC
GFRC
Woods


Electrical Conductivity (in units of reciprocal ohm-meters) (logarithmic scale)
10^8
10^4
1
10^{-4}
10^{-8}
10^{-12}
10^{-16}
10^{-20}
Metals
Semiconductors
Ceramics
Polymers

Global Material Issues

Challenges

- Non-efficient use of energy resources.
- The reserves of many economical minerals are diminishing. Copper (Cu), lead (Pb); Silver (Ag), Zinc (Zn) and Tin (Sn)...resources could be exhausted in our lifetime...
- Pollution and global warming (Environmental and Sociological issues).

Solutions

- Create designs that utilize materials in the most effective and efficient manner.
- Create materials that can be recycled; when the product has reached the end of its useful life.
- Search for other alternative renewable energy resources.

Cost and availability

- Cost and availability are very important factors which affect the selection and use of materials.
- For a product to be succeed in the market, it has to be made at an acceptable cost (the price that the buyer are willing to pay for the product or the service).
- The final cost of the finished product is influenced by many factors; including:
  - Raw material cost
  - Processing cost
  - Availability

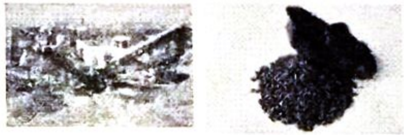
Cost of the raw material

- The cost of the raw material (accounts for about 50% of the total cost.
- The use of cheaper material have a significant effect on the final product cost.
- The cost of the raw material may change with time (for some materials, it is relatively unchanged over fairly long period of time but others are subjected to fluctuations). → Based on equations to estimate the optimal
- It is usual to see the cost of raw materials quoted per unit mass. However, in some occasions, the cost per volume may be used. ← Based on type of the material

→ Used these information to put the Plan for the manufacturing.

Processing cost

- The processing cost (in general, every process and heat treatment will give added value and increase the cost)
- Examples: The cost of alloys will be higher than the cost of unalloyed metals, for example, bronze (Cu-Sn) alloy is more expensive than pure copper. Due to manifacturing costs {Humens, energy, --}
- The cost of processed metal products such as sheets, plate, sections, and forging will be higher than those of ingot metal.


Cost of raw material


Processing cost

↳ look at every component of the process.

Availability

- The choice of a material for a particular application can be influenced by its availability.
- Example: In the major growth of railways in the 19th century most railway bridges in Britain were constructed of wrought iron. → has a carbon in it → with little percentage
- The principle is to use a material close to the source of material supply.

Example: Material selection for a tennis racquet frame?

Required properties: High strength, high stiffness, good damping characteristics and low weight.

manifactured as layers

Up to 1970s: racquet was made from laminated wood. (Drawback: it can absorb water which can lead to variations in performance and also can cause warping the frame).

problem need to be solved

In 1970s: frame was made from aluminum and steel (In spite of their good strength/weight ratio, they have low damping characteristics).

Problem need to be solved

In 1980s: frame was made from composite construction using glass or carbon fiber in a polyester or epoxy resin matrix. The new material has a high strength to weight ratio and good damping characteristics.

important

→ using smart material {piezo electric}, we test the properties of the racquet, to make sure that it is on the standard setuation

Example: Material selection for overhead electrical transmission wires

Required: high electrical conductivity

Metal candidate: silver, copper, gold and aluminum

Design concern: metal should have high purity as impurities cause a reduction in the electrical conductivity

How do we filter/select among the candidates?

List the advantages and disadvantages for each.

Gold and silver are very expensive for this application.

Copper is relatively more expensive than aluminum

Our choice: aluminum (drawback: very low tensile strength; this problem was solved by creating aluminum wires braided around a steel wire core to give strength).

Braided wire

Hashemite University

Faculty of Engineering
Industrial Engineering department

Engineering Materials
IE 110403352

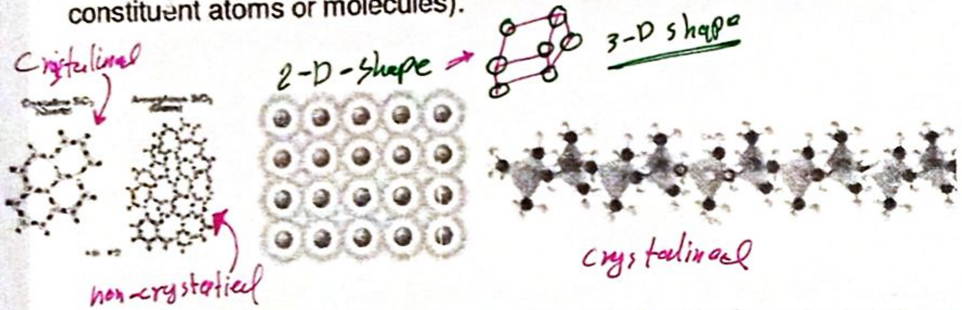
Dr. Morad Etier
morad.etier@hu.edu.jo

Chapter 2: Atomic Structure and Bonding

→ every ē has energy, which make him be in specific.

Introduction: Why study atomic structure and bonding?

- The final properties of any material depends on:
  - The manner in which the subatomic particles are assembled into atoms (Geometrical atomic arrangements)
  - The way in which various atoms are bonded to one another in the make-up of bulk materials (Bonding: Interaction that exist between constituent atoms or molecules).



Why polymers are electrical insulators and metal electrical conductors? → vatiabitty in the bondes

→ the difference in the stucture due to manifacturing method

→ All the metal is crystelliceal stucture

Definitions: Bohr model

Atomic number (Z) : Number of protons in the nucleus (ranges from 1 to 92)
Atomic mass (A) : Sum of masses of protons and neutrons within the nucleus.
Isotopes: when number of neutrons is variable in a certain atom for a certain element

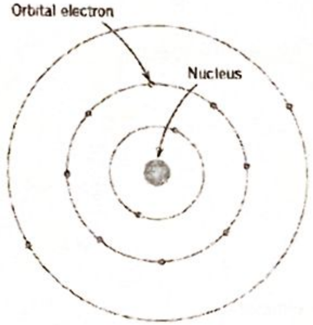


Figure 2.1 Schematic representation of the Bohr atom.

-An attempt to describe the electrons in atoms
- Electrons is assumed to revolve around the nucleus In discrete orbitals.

the Bohr model represents an early attempt to describe electrons in atoms, in terms of both position (electron orbitals) and energy (quantized energy levels).

⇒ Bohr's theoro only correct on the (H) electron ⇒ Thats why it doesn't fit

⇒ so, we found wave mechanical madel

Definitions: Quantum mechanical principle

free electron

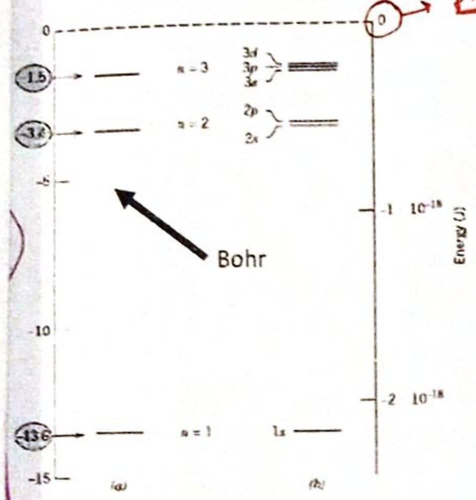


Figure 2.2 (*a*) The first three electron energy states for the Bohr hydrogen atom. (*b*) Electron energy states for the first three shells of the wave-mechanical hydrogen atom. (Adapted from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials*, Vol. I, *Structure*, p. 10. Copyright © 1964 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)

- The energy of the electrons is quantized
- Electron energy value may changed according to (absorption or emission of energy)

At zero energy, this is related to the unbound electron or free electron.

energy unit

Definitions: Wave mechanical model

energy unit

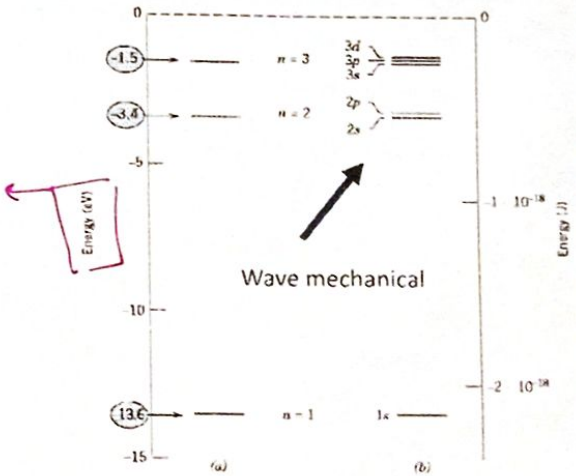


Figure 2.2 (*a*) The first three electron energy states for the Bohr hydrogen atom. (*b*) Electron energy states for the first three shells of the wave-mechanical hydrogen atom. (Adapted from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials*, Vol. I, *Structure*, p. 10. Copyright © 1964 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)

- In this model electron is considered to have both wave like and particle like characteristics
- Probability of the electron being in an orbital around the nucleus

Definitions: Bohr vs mechanical wave

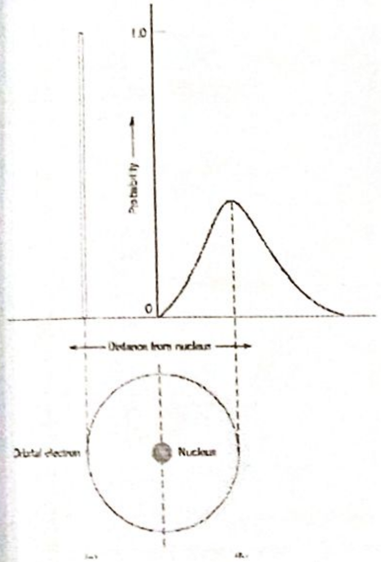


Figure 2.3 Comparison of the (*a*) Bohr and (*b*) wave-mechanical atom models in terms of electron distribution. (Adapted from Z. D. Jastrzebski, *The Nature and Properties of Engineering Materials*, 3rd edition, p. 4. Copyright © 1987 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)

Quantum numbers:

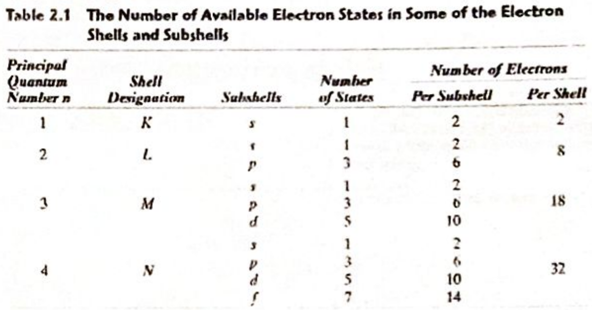


Table 2.1 The Number of Available Electron States in Some of the Electron Shells and Subshells

Principal Quantum Number n	*Shell Designation*	*Subshells*	*Number of States*	*Number of Electrons*	
				Per Subshell	*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	

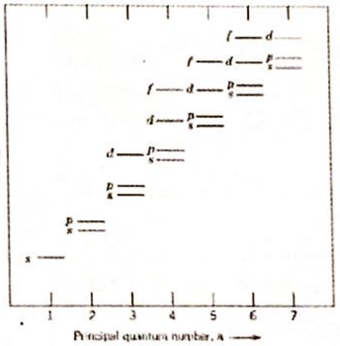


Figure 2.4 Schematic representation of the relative energies of the electrons for the various shells and subshells. (From K. M. Ralls, T. H. Courtney, and J. Wulff, *Introduction to Materials Science and Engineering*, p. 22. Copyright © 1976 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)

- Shells are specified by a principal quantum number n
- The number of energy states for each subshell is determined by the third quantum number, m_l
- *Associated with each electron is a spin moment, which must be oriented either up or down. Related to this spin moment is the fourth quantum number,* m_s

Pauli exclusion principle

s, p, d, and f subshells may each accommodate ,respectively, a total of 2,6,10,and 14 electrons

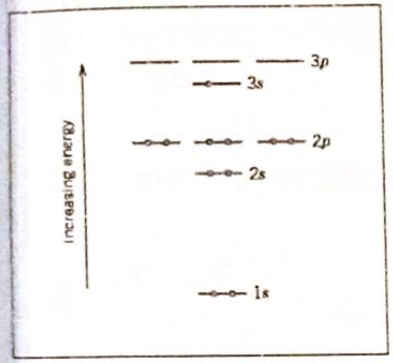


Figure 2.5 Schematic representation of the filled and lowest unfilled energy states for a sodium atom.

The valence electrons are those that occupy the outermost shell. These electrons are extremely important;, they participate in the bonding between atoms to form atomic and molecular aggregates.

→ our Goal

Survey of elements

المدار الأخير غير مكتمل

- Most elements: Electron configuration not stable.

Element	Atomic #	Electron configuration
Hydrogen	1	$1s^1$
Helium	2	$1s^2$ (stable)
Lithium	3	$1s^22s^1$
Beryllium	4	$1s^22s^2$
Boron	5	$1s^22s^22p^1$
Carbon	6	$1s^22s^22p^2$
...		...
Neon	10	$1s^22s^22p^6$ (stable)
Sodium	11	$1s^22s^22p^63s^1$
Magnesium	12	$1s^22s^22p^63s^2$
Aluminum	13	$1s^22s^22p^63s^23p^1$
...		...
Argon	18	$1s^22s^22p^63s^23p^6$ (stable)
...	...	...
Krypton	36	$1s^22s^22p^63s^23p^63d^{10}4s^24p^6$ (stable)

مستقرة

الموجود داخل المدار الرئيسي الغير كامل هو valence ē

When you start "filling" the orbitals with electrons there is a certain sequence, from the lowest (more stable) orbitals to the highest energy.

For almost all the atoms, the sequence is this:

1s
2s 2p
3s 3p 3d
4s 4p 4d 4f
5s 5p 5d 5f
6s 6p 6d
7s

and cut this array in diagonal. It will provide you with a way to "fill" with electrons the orbitals of most atoms. here's the sequence:
1s 2s 2p 3s 3p 4s 3d 4p 5s 4d 5p 6s 4f 5d 6p 7s 5f 6d → the correct schedule to put the ēs

↳ depends on the energy

- Why? Valence (outer) shell usually not filled completely.

$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6$

الترتيب الصحيح

Adapted from Table 2.2, *Callister 7e.*

Electron Configurations

- 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: C (atomic number = 6)

$1s^2 \boxed{2s^2\ 2p^2}$ ← valence electrons

1	2
K	L
2	8(2+6)

Electronegativity

Electropositivty

- Electronegativity is chemical property that describe the ability of atoms of the element to attract electrons of atoms of another element.

give

to

Electropositive elements, indicating that they are capable of giving up their few valence electrons to become positively charged ions.

الذي يؤثر على ال electro negativity

Electronegativity is affected by both its atomic number and the distance that its valance electrons reside from the charged nucleus.

• الإلكترونات القريبة ع النواة Energy عالية :-

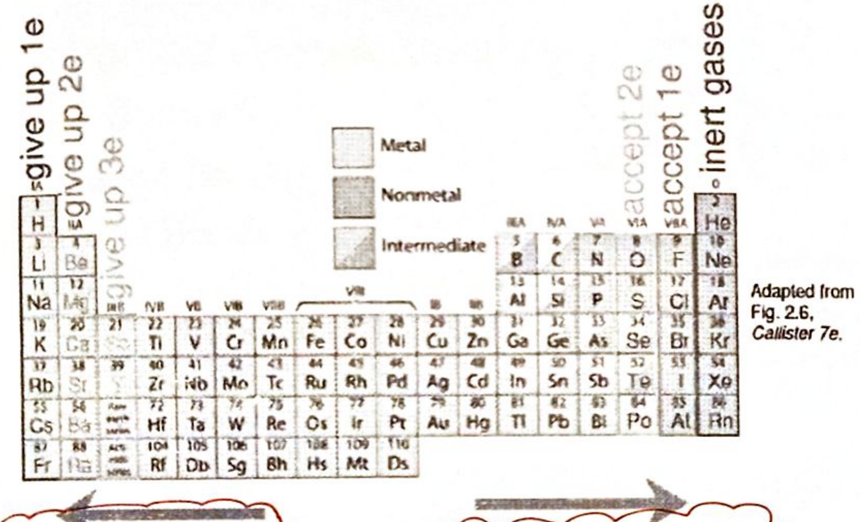
←

* قوة الرابطة تعتمد على كمية الطاقة اللازمة لفك
هذه الرابطة ⇐ الفرق بين الكهروسلبية

* كلما زاد الفرق بين Electronegativity بين عنصرين الرابطة
زادت قوة الرابطة

The Periodic Table

- Columns: Similar Valence Structure



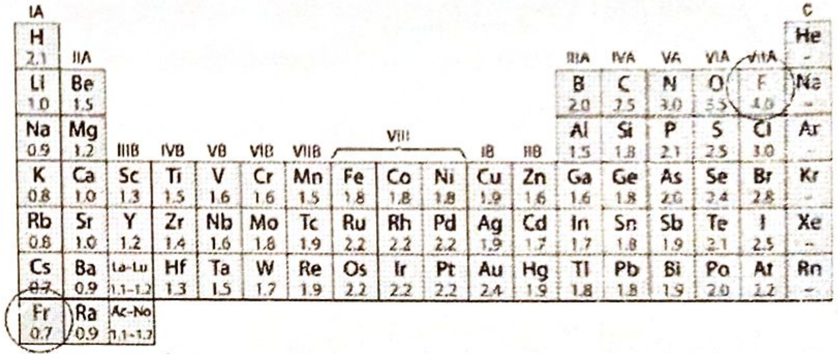
Adapted from Fig. 2.6, *Callister 7e.*

Electropositive elements: Readily give up electrons to become + ions.

Electronegative elements: Readily acquire electrons to become - ions.

Electronegativity

- Ranges from 0.7 (francium) to 4.0 fluorine
- Large values: tendency to acquire (gain) electrons.



IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIII			IB	IIB	IIIA	IVA	VA	VIA	VIIA	0
H 2.1																	He -
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0	Ne -
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0	Ar -
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.8	Ni 1.8	Cu 1.9	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8	Kr -
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5	Xe -
Cs ~~0.7~~	Ba 0.9	La-Lu 1.1-1.2	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Tl 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2	Rn -
Fr 0.7	Ra 0.9	Ac-No 1.1-1.7															

Smaller electronegativity

Larger electronegativity

Adapted from Fig. 2.7, *Callister 7e.* (Fig. 2.7 is adapted from Linus Pauling, *The Nature of the Chemical Bond*, 3rd edition, Copyright 1939 and 1940, 3rd edition. Copyright 1960 by Cornell University.

Chemical Bonding

- Interatomic / Primary Bonding
  - Ionic Bonding
  - Covalent Bonding
  - Metallic Bonding for lequid forms
- Intermolecular / Secondary Bonding
  - Hydrogen Bonds
  - Van der Waal's

{ all the secondary Bonding are vander waals }

Primary bonds are strong; Secondary bonds are weak ★

Ionic Bonding

- Occurs between +ve and -ve ions. → particle charge
- Requires electron transfer
- Large difference in electronegativity required.
- Predominant bonding in Ceramics

قوة الرابطة تعتمد على الفرق في الكهروسلبية

Ion (cation and anion)

Ion: a charged particle, the net charge may be positive or negative depending on whether or not electrons are lost or gained.

★ Cation: positive ion ★

★ Anion: negative ion ★

→ required in every ionic bond

→ Ceramics → depends on ionic bond

Metal + non-metal

Most popular for ionic bonding

* الـ Vanelar Waal's ← هي القوة ما بين كل NaCl و NaCl الآخر

Ionic bond = metal + nonmetal

metal ↑ donates electrons

nonmetal ↑ accepts electrons

Dissimilar electronegativities (Mg:1.2; O:3.5)

ex: MgO

↓ kind of ciramic {powder}

Mg $1s^2\ 2s^2\ 2p^6\ 3s^2$

1	2	3
K	L	M
2(2)	8(8)	18(2)

O $1s^2\ 2s^2\ 2p^4$

1	2
K	L
2(2)	8 (6)

Mg^{2+} $1s^2\ 2s^2\ 2p^6$

1	2
K	L
2(2)	8(8)

O^{2-} $1s^2\ 2s^2\ 2p^6$

1	2
K	L
2(2)	8(8)

these bond depends on coloumb force

* داخل الرابطة الأيونية :-
تتحكم الكهروسلبية في قوة الرابطة + عدد الذرات + عدد الالكترونات
المدار الأخير

Ionic bond → الرابطة الأقوى

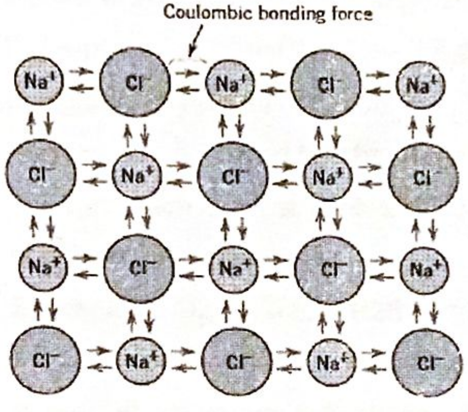
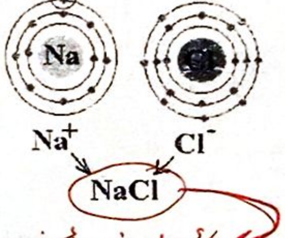


Figure 2.9 Schematic representation of ionic bonding in sodium chloride (NaCl).



دلالة على فيه أخذ وعطا

Na

$1s^2 2s^2 2p^6 3s^1$

Cl

$1s^2 2s^2 2p^6 3s^2 3p^5$

Na^+

$1s^2\ 2s^2\ 2p^6$

Cl^-

$1s^2 2s^2 2p^6$
$3s^2\ 3p^6$

{non-polar}

Covalent Bonding- Types

ثاني أقوى رابطة

Single covalent bond (only one shared pair of electrons), i.e.

Cl_2 $Cl - Cl$

Multiple (more than one pair of electrons shared between the atoms) → Multiple {single covalent bond} $H-\overset{H}{\underset{H}{C}}-H$

Double: (two pair of electrons shared between the atoms), i.e.

O_2 $O = O$

Triple: (three pair of electrons shared between the atoms), i.e.

C_2H_2 $H\text{-}C{\equiv}C\text{-}H$

$Cl: 2s^1 2s^2\ 2p^6 \boxed{3s^2 3p^5}$

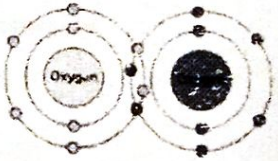
Covalent Bonding - Concept

How do we achieve the stable arrangement of electrons in this type of bonding? Electron sharing

Example 1: $2Cl \rightarrow Cl_2$, $Z_O = 17$ this bond can be designated by (Cl:Cl or Cl-Cl)*

The bond is achieved by sharing a pair of electrons, 1e⁻ from each enter a joint orbit around both nuclei (single covalent bond).

Example 2: O_2, $Z_O = 8$, $1S^2 2S^2 2P^4$



Each O atom need $2e^-$ to reach the steady state

2 pair of electrons are shared between the two adjacent atoms (double covalent bond)

* Pair of dots or hyphen represents a pair of electrons shared between adjacent atom (one covalent bond)

Examples:-

N_2 ↓ {Triple covalent bond}

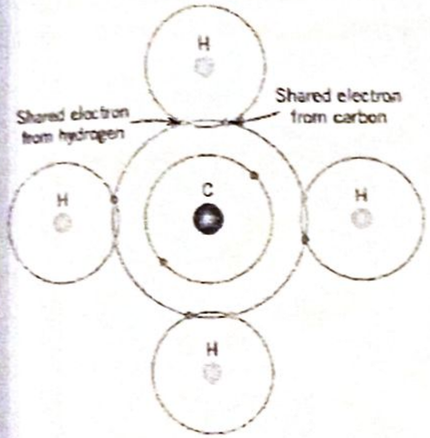


Figure 2.10 Schematic representation of covalent bonding in a molecule of methane (CH_4).

Multiple single covalent bond

* الرابطة الأيونية و المشتركة يمكن أن تكون بين أكثر من نوع من الذرات

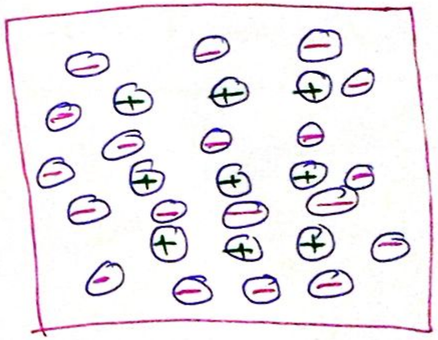
* تكون الرابطة بين نوع واحد من الذرات

ذات قوى رابطة

The Metallic Bond → خاصة بالمعادن

- In metals, number of valence electrons in each atom is small (1, 2, or 3). Therefore, it is not possible to fully satisfy the stability condition as in the ionic or covalent bonds.
- The outer shell electrons, at certain points in their orbits, are attracted as much by one nucleus as by another
- The valence electrons follow a complex paths around many nuclei (electron clouds)
- Valence electrons are shared by all atoms in the assembly
- Valence electron are extremely mobile, which give the rise to the good electrical and thermal conductivities.

that's give us high conductivity

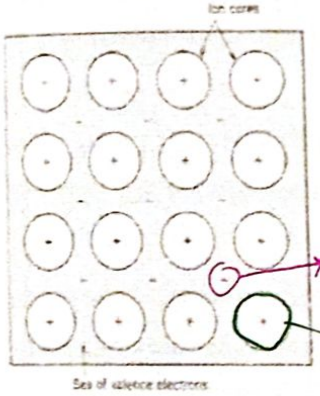


* الروابط الأساسية :-

① ionic bonds
② covalent bonds
③ Metallic bonds

The Metallic Bond

In the metallic bonding these electrons (valance electrons) are not bound to any particular atom in the solid, and they are free to move through the entire metal?



valenced electron

the whole atom without valenced electrons

Ion core: the remaining non valence electrons and atomic nuclei. The net positive charge of the ion cores equal in magnitude to the total valence electron charge per atom.

Approximation to the bonding scheme (behaviour)

complex path

H → N
H → O
H → F

as well as van der waal's but stronger

Secondary Bonds

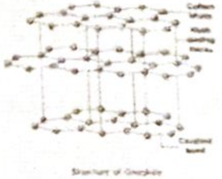
Kind of van der waal's bonds

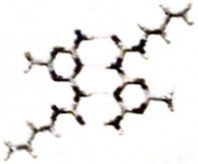
رابع أقوى رابطة

Hydrogen bond: Electronegative atom is covalently bonded to hydrogen which is also bonded to another electronegative atom, Example: H_2O.

خامس أقوى رابطة

Van der Waal's: Many molecular compounds are polarized to some extent, there is a weak electrostatic attractive force between the molecular dipole. Examples: clay minerals and graphite,





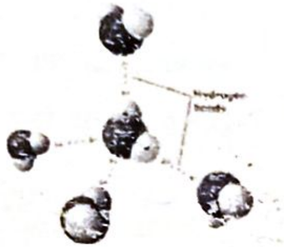
* أي رابطة جزيئات ← Von der Waal's

Secondary Bonds

1) The H_2O molecule is polar, the 2 hydrogen ends being (+ve) relative to the non bonding orbitals f the oxygen atom (-ve) .

2) There is a strong force of attraction between the the hydrogen and the (-ve) ends of adjacent nolecule

The hydrogen bond does not only occur in water and Ice, but in a number of polymeric materials too.



[illegible]	[illegible]
Hydrogen	0.2
Van der Waal's	0.002-0.1
Ionic bond/NaCl	6.5

Atomic and molecular bonding energy

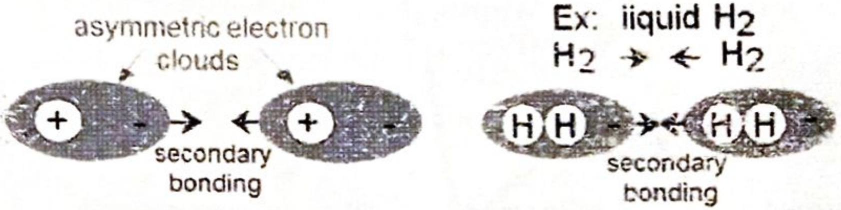
Examples of polymeric materials that have hydrogen bond: (1) bonds between polyamide (nylon) molecule. (2) bonds in cellulose and polyvinyl alcohols.

Secondary Bonds

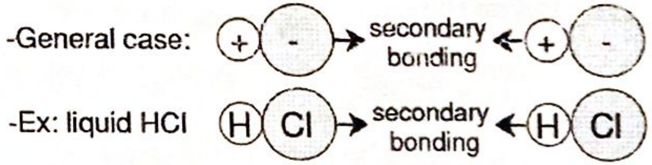
Arises from interaction between dipoles

- Fluctuating dipoles

Ex: liquid H_2



- Permanent dipoles-molecule induced



Adapted from Fig. 2.13, *Callister 7e.*

Adapted from Fig. 2.14, *Callister 7e.*

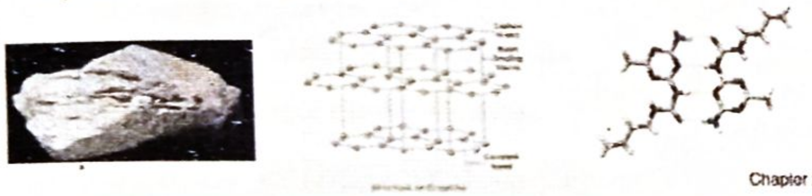
*Bond Energy → الطاقة اللازمة لفك الرابطة

* لما يكون ال Centers أقرب ما يمكن على بعض بتكون أعلى تنافر بين الذرات

Secondary Bonds

Hydrogen bond: Electronegative atom is covalently bonded to hydrogen which is also bonded to another electronegative atom, Example: H_2O.

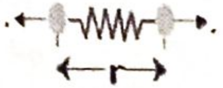
Van der Waal's: Many molecular compounds are polarized to some extent, there is a weak electrostatic attractive force between the molecular dipole. Examples: clay minerals and graphite,



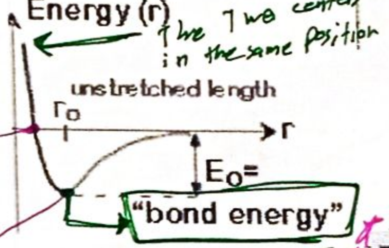
PROPERTIES FROM BONDING:

T_M

- Bond length, r
- Melting Temperature, T_m



- Bond energy, E_o

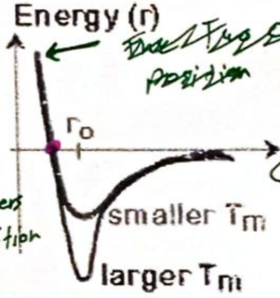


The Two centers in the same position

بلشى التجاذب بين الذرتين

optimal point

قبلها في تجاذب و لكن غير كافية لإنشاء الرابطة



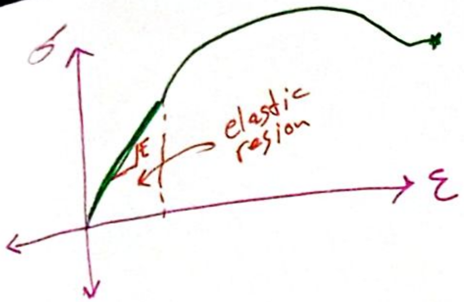
~~Bond Two centers in the same~~ position

r → المسافة

ما بين ال Atoms

{ما بين ال Centers}

T_m is larger if E_o is larger



* كلما زادت قيمة E
⇐ تكون مقاومة المادة
للـ load أعلى

⇐ يعود ذلك لقوة
الروابط للمادة

$\alpha = \frac{\varepsilon}{\Delta T} = \frac{\frac{\Delta L}{L}}{\Delta T}$

→ Thermal expantion coefficitont

→ unit: $\{1/C\}$ أو $\{K^{-1}\}$

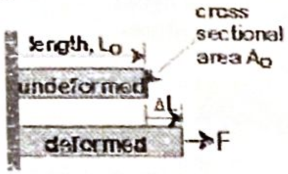
* كلما زادت قيمة Thermal expation
تكون قوة الروابط بين المادة أقل
⇐ Bond energy أقل ⇐ Melting Paint أقل

PROPERTIES FROM BONDING: E

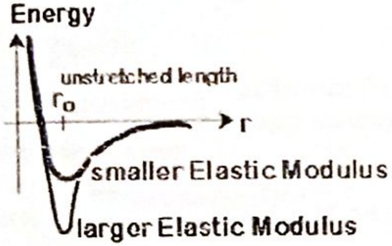
- Elastic modulus, E

Elastic modulus

$\frac{F}{A_o} = E\frac{\Delta L}{L_o}$



- E ~ curvature at r_o



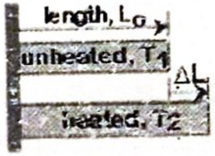
E is larger if E_o is larger.

PROPERTIES FROM BONDING: α

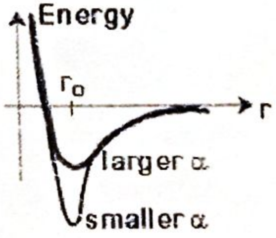
- Coefficient of thermal expansion, α

coeff. thermal expansion

$\frac{\Delta L}{L_o} = \alpha(T_2 - T_1)$



- α ~ symmetry at r_o



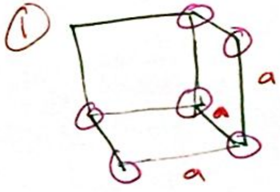
α is larger if E_o is smaller.

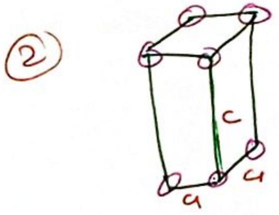
SUMMARY: PRIMARY BONDS

Ceramics (Ionic & covalent bonding): المعظم	Large bond energy large T_m large E small α
Metals (Metallic bonding):	Variable bond energy moderate T_m moderate E moderate α
Polymers (Covalent & Secondary): المعظم	Directional Properties Secondary bonding dominates small T small E large α

Chapter 3: Crystalline Structure

مواد ال Atoms فيها مرتبة





and 5 More Types

Introduction

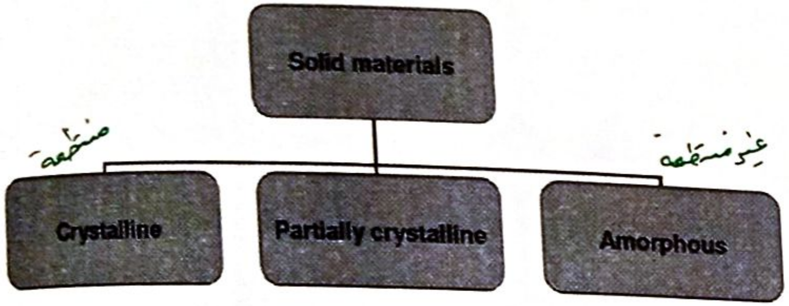
Issues To Address...

- How do atoms assemble into solid structures?
- Know the difference between crystalline and amorphous solids.
- Know the name and definitions of the seven crystal system.
- How does material properties vary with the its crystal structure?
- Understand Miller notations and be able to derive the Miller indices for planes and directions within crystal unit cells.
- Understand the concept of the unit cell and be able to sketch the unit cells of the body centered cubic, and face centered cubic.

3 أرقام تصف ال plane اللي إحنا بنشتغل فيه

التقسيم على حسب ترتيب ال Atom

Introduction



The classification is based upon the arrangement of the constituent atoms or molecules of the substance after solidification.

Does they form a regular pattern?
Is this pattern repetitive or symmetrical?

الشروط عشان أحكي عن المادة
{crystailine}

← تنطبق هذه الشروط على معظم المواد

Why study crystal structure?

- **Crystalline structure:** The constituent atoms or ions are arranged in ① regular, ② repetitive and ③ symmetrical array.
- Many solid materials are crystalline in nature.

بعض ال ceramics
مش crystailine لكن
الأغلب crystalline

- The properties of a material are determined by the type of the crystal structure. This is particularly true for metals.

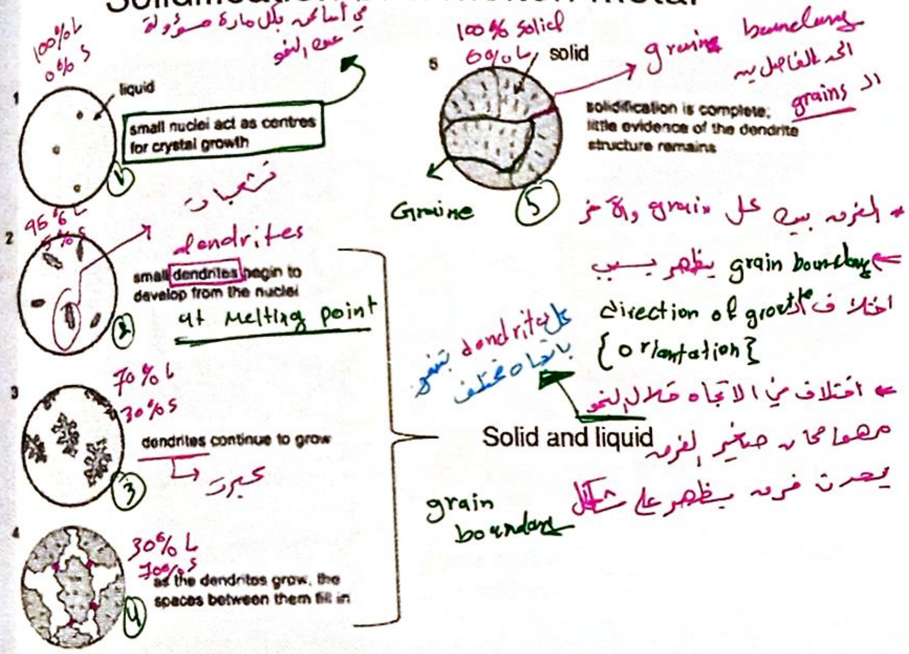
Chemical
Electrical
Thermal
Optical
…

* عشان نصنع أي Metal لازم نوصل الـ Melting Point
أعلى من
عشان يكون liquid ، وتشكلت بالتبريد

---

* كل طريقة تبريد ينتج عنها structure مختلف عن الآخر

Solidification of a molten metal



* الغرفة بين كل grain والآخر
⇐ grain boundary يظهر بسبب
اختلاف direction of growth
{orientation}
⇐ اختلاف في الاتجاه خلال النمو
كل dendrite تنمو باتجاه مختلف
مهما كان صغير الفرق
يحدث فرق يظهر على شكل grain boundary

Stages of metal solidification and formation of polycrystalline material

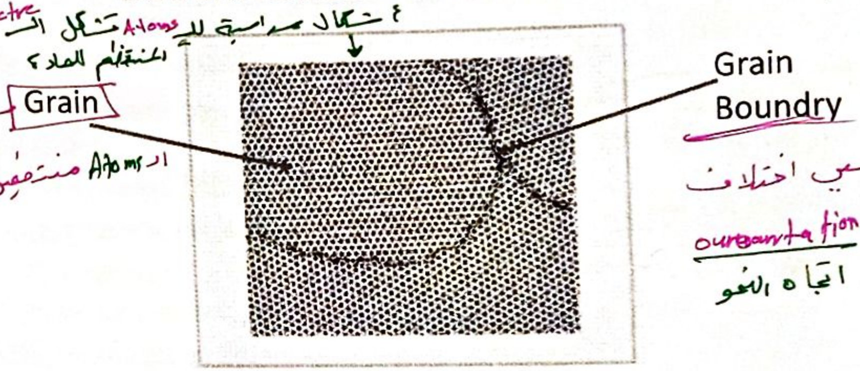
during the solidification ~~the~~ the tem constant

② + ③ + ④ + ⑤

* طرق التبريد :- ① الهواء ② مياه وملح ⟨الأسرع⟩ ③ رمل
④ زيت ⑤ أنه نتركها بدرجة حرارة الغرفة
⑥ فرن الغرفة واتركها فيه

* التصنيع بالوضع الطبيعي
Poly cristylined Material
بنقدر نتحكم بالمادة أكثر

Solidification of molten metal



- The atoms pack together in an orderly and repetitive manner.
- At the boundaries between the grains, the regular pattern breaks down, as the pattern changes from the orderly pattern of one grain to that of the next.

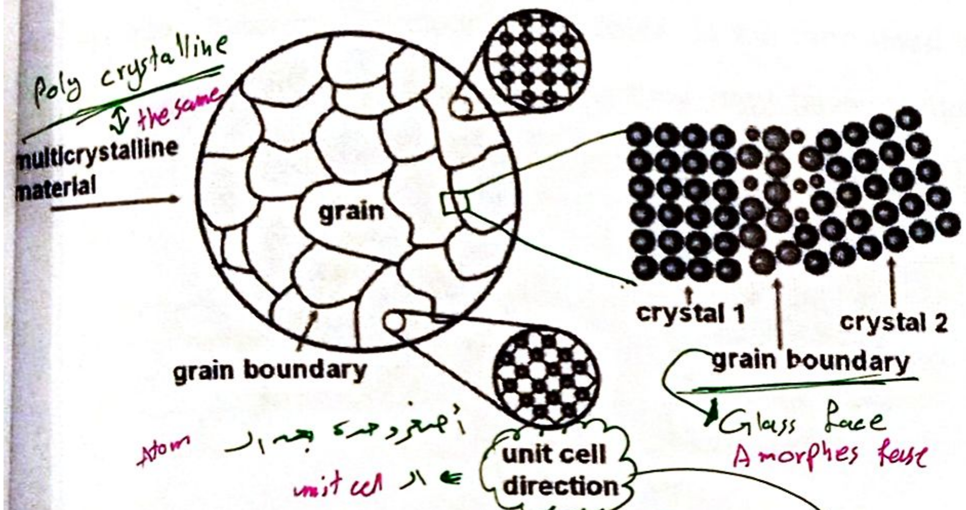
* Single crystal → Grain واحدة] → تستخدم لصنع قطع معينة منها الـ pressure
بنفس الـ orientation

* جزء من ال Grain ⇐ crystal

* بالعادة ال Metals تكرن بالمايكرومتر

* ال Graine تحتوي على مجموعة كبيرة من ال Atoms

Polycrystalline material



Atom أصغر وحدة بجسم ال

unit cell ال ⇐

Polycrystalline : many **crystallites** of varying size and orientation
Most inorganic solids are polycrystalline, including all common metals and many ceramics.

repeatitive

يختلف من مادة لمادة

وحدة مهمة في عالم المواد

Å → 10^{-10} m

Crystalline structure

- **Crystalline structure:**

The constituent atoms or ions are arranged in regular, repetitive and symmetrical array. The regularity of the structure may be termed as long range order, or short range order.

- **Long range order:** عدد كبير من ال crystals

  The same symmetrical pattern of atoms or ions exist over large distances within the material.

- **Short range order:** عدد قليل من ال crystal
  - لو وصلو –Repetition is only over a range 10-20 atoms.
  - 100-200, -- –Local groups of atoms or ions may be in a symmetrical pattern.
  - still short range order –The relationship between these local groups may not be regular.

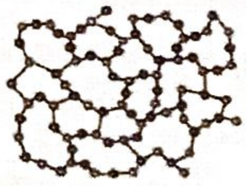
Amorphous structure

- **Amorphous**, meaning literally **without form**, is the term used to describe non crystalline structures, even they may have a short range order (Short range order is found in many inorganic glasses).

أهم مثال


Crystalline structures


Short range order


Non crystalline structures

* أسرع طريقة التبريد بالماء والثلج

* التركيب الزجاجي ← non crystalline structure

Structure of solid materials

- Metals and ceramics are crystalline solids.
- In many polycrystalline ceramics there is a frequently a glassy phase in the space between crystal grains.
- Many polymer materials show a greater or lesser degree of crystallinity but others are amorphous.
- Inorganic glasses have amorphous structure, even though they have the same composition as ceramics.

Solidification and crystallization

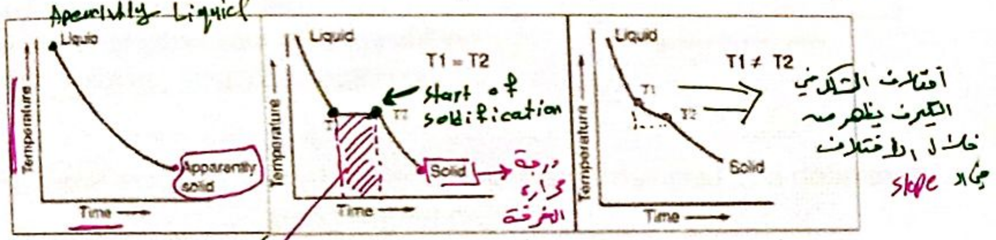
Once the material is allowed to cool slowly from the liquid state , the cooling curve (Temp. Vs Time) obtained can be:

Continuous cooling curve: (glassy material)

- No definite solidification temperature.

Discontinuous cooling curve: (crystalline material)

- Definite unique solidification temperature for pure metal.
- Solidification occurs over a range of temperatures for alloys.



Amorphes Material

for pure Metal

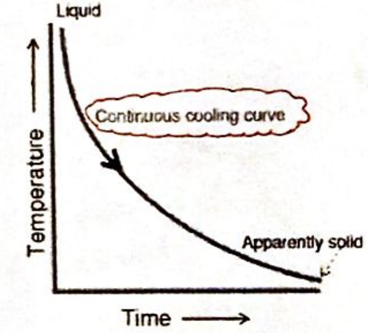
Soldification resion constant tem

two crystalline Material mixed withe each other

Cooling curve for a glassy material

As the temperature falls upon cooling:

- A steady **decrease in the kinetic energy** of the atoms or molecules that make up the liquid.
- A steady **increase in the viscosity** of the fluid.
- The atoms or molecules present still have the same type of **random arrangement** that existed in the true fluid state.



What are the changes occur in material during cooling?

True fluid	Viscous fluid	Apparent solid (Amorphous solids or glasses)

* [illegible] كلما ارتفع درجة الحرارة تزيد اللزوجة

Cooling curve for a pure crystalline material

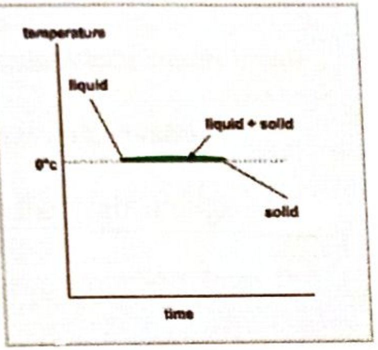
s the temperature falls upon cooling:

There is a definite freezing or solidification point

At the freezing temperature:

- The atoms cease their random movement.
- They tend to 'stick' together in relatively fixed positions in a regular pattern.

- The atomic motion does not cease abruptly upon solidification.
- The atoms or molecules in a crystalline structure vibrate about fixed positions.



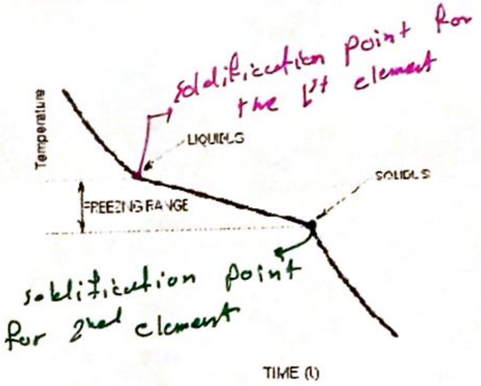
Cooling curve for pure water

In crystalline material, atoms or molecules are arranged in a definite symmetrical pattern.

Cooling curve of a crystalline material (alloy)

As the temperature falls upon cooling:

1) There is no specific freezing temperature.
2) Material freeze or solidify upon a range of temperatures.
3) The resultant structure is crystalline solid.
4) The same mechanism of pure solid solidification applies.



Cooling curve for an alloy

In crystalline material, atoms or molecules are arranged in a definite symmetrical pattern.

Latent heat

As the liquid solidify, the material changes from a **high energy state** (random motion of atoms or molecules) to a much **lower energy state** (and vibrate about a point within a crystal).

Latent heat is the difference between the high energy state and the low energy state, it is the energy emitted from the material at the freezing temperature.

ترتيب {رصة}

Materials and Packing

Crystalline materials...

- Atoms pack in periodic, 3D arrays
- Typical of:
  - 1 -metals
  - 2 -many ceramics 95%
  - 3 -some polymers

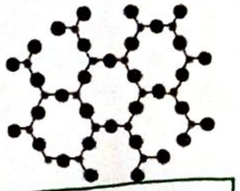
Noncrystalline materials...

- Atoms have no periodic packing
- Occurs for:
  - 1 -complex structures
  - 2 -rapid cooling

الترتيب بيحتاج الى الوقت كما ذكرنا في الكيرف السابقه وفي التبريد السريع لا يتم تحصيل هذا الوقت ← noncrystalline Material

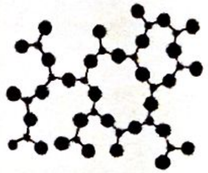
لمعظم الحالات

"Amorphous" = Noncrystalline



مثال على

crystalline SiO_2



noncrystalline SiO_2

• **Si** ● **Oxygen**

Silicon dioxide

Adapted from Fig. 3.22(a), *Callister 7e.*

Adapted from Fig. 3.22(b), *Callister 7e.*

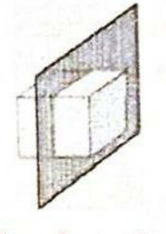
crystillized Material ⇐ one axis / one plane of symmetry علي أقل ←

Symmetrical structure

- A shape is said to be symmetrical if it posses one or more elements of symmetry.
- Some of the elements of symmetry: planes, axes of symmetry.
- The degree of symmetry in a shape depends on the number of symmetrical elements that exist in that shape.
- A shape of low symmetry may has only one plane of symmetry.
- A highly symmetrical shape, such as the cube, will contain several planes and axes of symmetry.

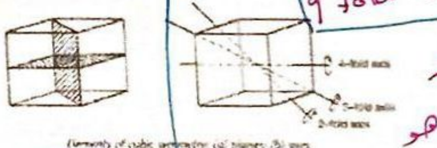
Plane of symmetry and axis of symmetry

- **Plane of symmetry:**
  - A shape is said to be symmetrical about a plane if the plane divides the shape into either two identical halves, or into two halves that are mirror images of one another.
- **Axis of symmetry:**
  - If the shape can be rotated about an axis so that the shape occupies the same relative position in space more than once in a complete revolution then such an axis is termed an axis of symmetry.
  - The line in a plane divides the figure into two such parts that one part, when folded over along the axis, shall coincide with the other part.



Plane of symmetry

Axis of symmetry



Elements of cubic symmetry: (a) planes; (b) axes.

4 fold Axis

بعمل دوران للشكل وبعد زاوية معينة برجع زي ماهو

Axis of symmetry ⇐ Revelution

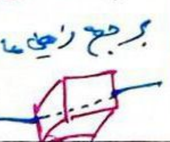
المكعب الشكل الوحيد الذي يحوي 13 Axis of symmetry

2 fold Axis

عددهم ← 6

⇐ بلفه 180 درجة برجع زي ما هو

ex:

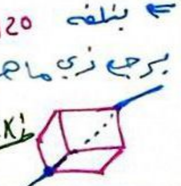


3 fold Axis

عدد هم ⇒ 4

⇐ بلفه 120 درجة برجع زي ماهو

ex:



طرفيه أربع مرات و رجع نفس الشكل

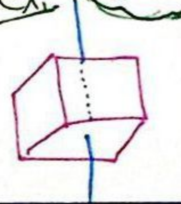
4 folded Axis for the cube

⇒ عددهم 3

ولاقيته تلاتي أكثر

بلفه 90 درجة برجع زي ما هو

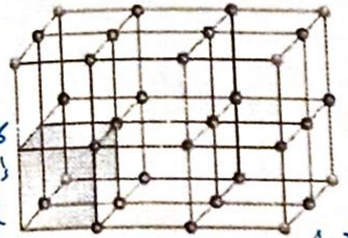
ex:



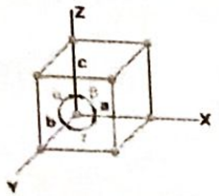
إختلاف العناصر المتشابهة في ال unit cell شكل ولكن تختلف بالأحجام
a, b, c

ال unit cell تختلف بالأبعاد الثلاثة والزوايا بينهم
a, b, c
α, β, α

Space lattice and unit cell


كل مادة لها unit cell

Representation of space lattice and unit cell



Representation of dimensions of a unit cell

تعرف ب 3D طول وعرض وارتفاع

مجموعة من ال Atom

Unit cell: the smallest building block of atoms that are arranged in three-dimensional space (unit cell describes the spatial arrangement of atoms).

When the unit cell is repeated in different directions, it will form what is called crystal lattice or space lattice.

Crystal lattice or space lattice is a regular arrangement of the constituent particles of a crystal in a three dimensional space.

مجموعة من ال unit cell

Crystal Systems

Unit cell: smallest repetitive volume which contains the complete lattice pattern of a crystal. The unit cell geometry is completely defined in term of six parameters (Lattice Parameters): three edge lengths, and three inter-axial angles.

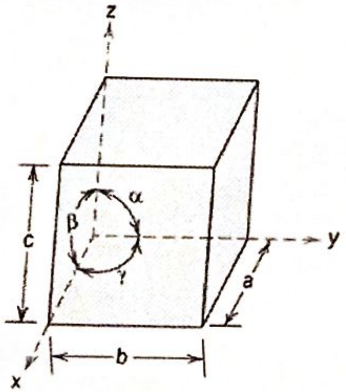


Fig. 3.4, *Callister 7e.*

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

7 crystal systems

Crystal systems

أساس علم المواد مهم جداً

There are seven crystal systems. These are:

(1) Triclinic

(2) Monoclinic

(3) Rhombohedral

(4) Hexagonal

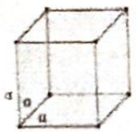
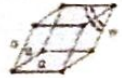
(5) Orthohombic

(6) Tetragonal

(7) Cubic

مهم جداً

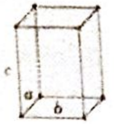
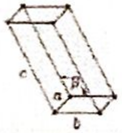
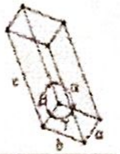
Crystal systems

Crystal System	Axial Relationships	Interaxial Angles	Unit Cell Geometry
① Cubic	$a = b = c$ $a = b = c$	$\alpha = \beta = \gamma = 90°$ $\alpha = \beta = \gamma = 90°$	
Hexagonal الوحيد اللي مش مشتقه من ال Cubic	$a = b \neq c$ $\boxed{a = b} \neq c$ ← القاعدة مسدسة	$\alpha = \beta = 90°, \gamma = 60°$ $\alpha = \beta = 90, \gamma = 60$	
② Tetragonal	$a = b \neq c$ $a = b \neq ⓒ$	$\alpha = \beta = \gamma = 90°$ $\alpha = \beta = \gamma = 90$	
③ Rhombohedral (Trigonal)	$a = b = c$ $a = b = c$	$\alpha = \beta = \gamma \neq 90°$	

★ أغلب المعادن مشتقة من ال Cubic و ال Hexagonal

مهم جداً

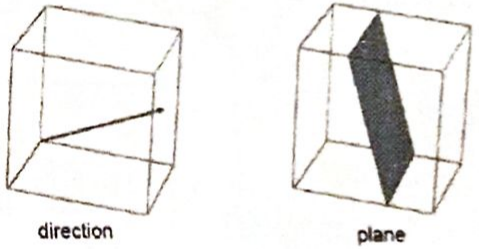
Crystal systems

Crystal System	Axial Relationships	Interaxial Angles	Unit Cell Geometry
Orthorhombic ④	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$	
Monoclinic ⑤	$a \neq b \neq c$	$\alpha = \gamma = 90° \neq \beta$	
Triclinic ⑥	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90°$	

⑥ + ⑤ + ④ + ③ + ② + ①

Cubic مشتقات من الـ

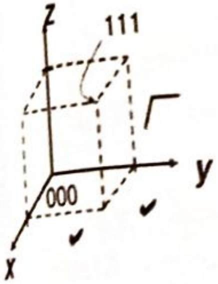
Crystallographic planes and directions



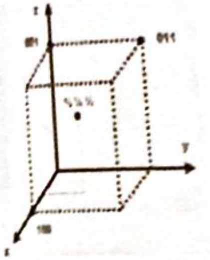
- It is often necessary to be able to specify certain directions and planes in crystals.
- Many material properties and processes vary with direction in the crystal.
- Directions and planes are described using three integers, Miller indices.

لغة خاصة في علم المواد 3 أرقام، كل رقم لها
معنى تصف الـ material والأشكال الظاهرة للرقم لها معاني
معروفة ضمن دراسة علم المواد

Point Coordinates



Point coordinates for unit cell corner are (111)



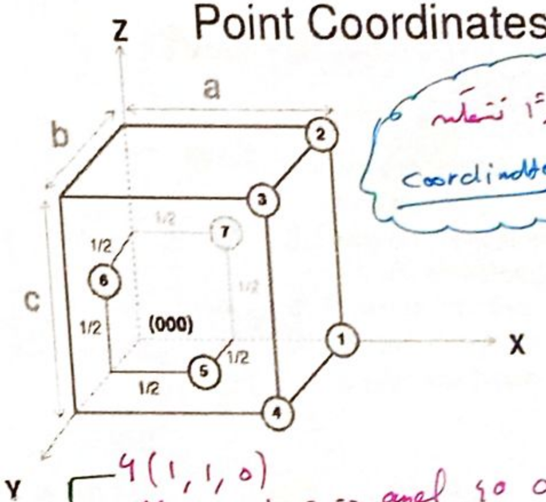
Point coordinates for unit cell center are:

a/2, b/2, c/2   (½½½)

Translation: integer multiple of lattice constants → identical position in another unit cell

---

Point Coordinates



• مو بعد ١ نشتغل
مع ال coordinates

4(1,1,0)
7(½,0,½) ... and so on...

notes-

No Comas

Give the coordinate for the atoms 1, 2, 3, 4, 5, 6 and 7 within the unit cell (for this unit cell a = b = c = 1 unit).

General Rules for Lattice Directions, Planes & Miller Indices

- Miller indices used to express lattice *planes* and *directions*
- x, y, z are the axes (on arbitrarily positioned origin)
- a, b, c are lattice parameters (*length of unit cell along a side*)
- h, k, l are the Miller indices for planes and directions - expressed as planes: (hkl) and directions: [hkl]

① integers num , ② negative above the num / ③ no commas

④ [0-9] → فقط

very imported rules to Miller indices

- Conventions for naming
  - There are NO COMMAS between numbers
  - Negative values are expressed with a bar over the number
    - *Example: -2 is expressed* $\overline{2}$
- Crystallographic direction:
  - [123]
  - [100]
  - … etc.

[direction vector]

(crystallografic Plane)

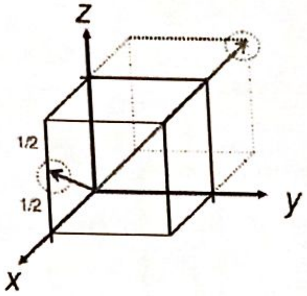
{ family of crystallografic planes }

< family of direction >

أنواع الأقواس
المتضمنة في
Miller indices ال

[ ]

Crystallographic Directions



Algorithm

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

ex: 1, 0, ½ => 2, 0, 1 => [201]

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

Families of directions <*uvw*>

→ Vector in Miller indices:

[h k l]

Crystallographic direction, [uvw]

Vector 1:

Start: 1, 0, 1

End :0, 0 ,0

End – start = (0 -1), (0 – 0), (0 -1)

End – start = -1, 0 , -1

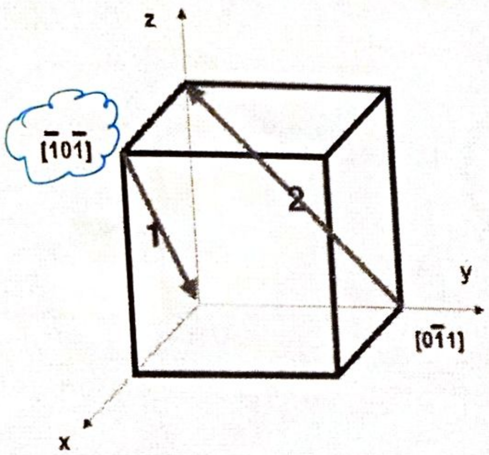
Vector 2:

Start: 0, 1, 0

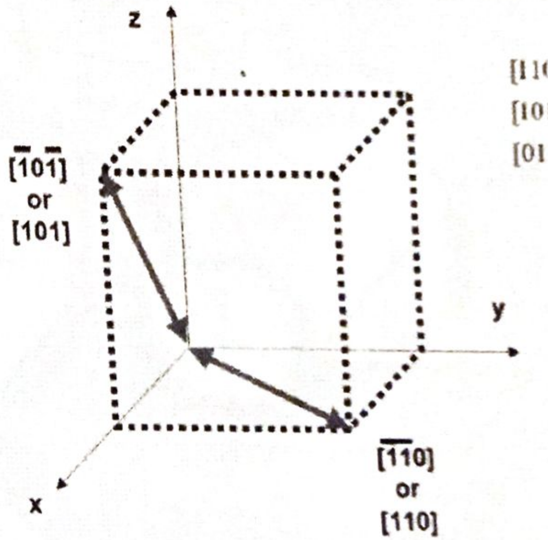
End :0, 0 ,1

End – start = (0 -0), (0 – 1), (1 -0)

End –start = 0, -1, 1

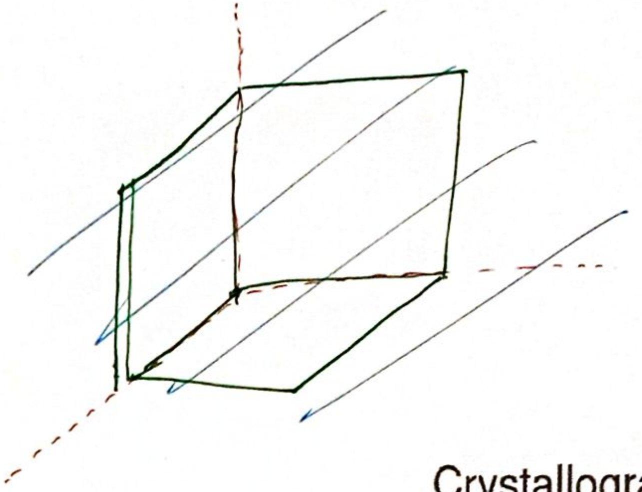


Family of crystallographic directions <uvw>



<110>

[110],[$\bar{1}$10],[1$\bar{1}$0],[$\bar{1}\bar{1}$0]
[101],[$\bar{1}$01],[10$\bar{1}$],[$\bar{1}$0$\bar{1}$]
[011],[0$\bar{1}$1],[01$\bar{1}$],[0$\bar{1}\bar{1}$]



Crystallographic directions

Vector 1:

Start: 0, 0, 0

End: ½, 1, ½

End – Start = ½, 1, ½

[121]

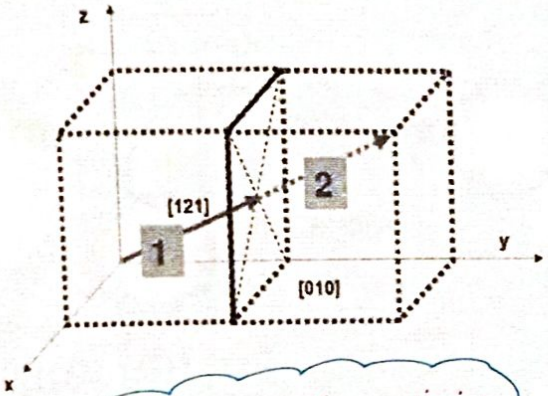
Vector 2:

Start: ½, 1, ½

End: 1, 2, 1

End – Start =½, 1, ½

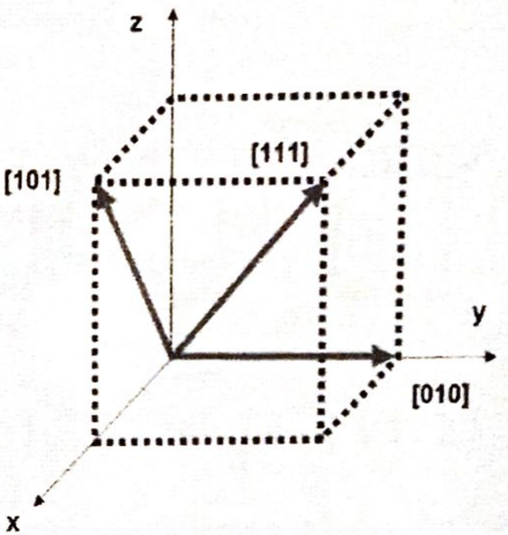
[121]



← نتخلص من الكسور بالضرب بالعامل المشترك

← الهدف من الـ vector هو تحديد اتجاه لذلك طلع الـ 2Vectors نفس الدلالة لأنهم نفس الإتجاه

Crystallographic Directions

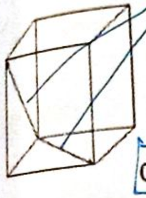


< >

Families of directions

- Equivalence of directions

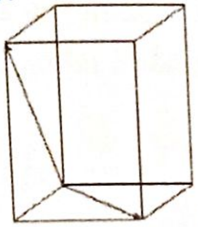
family of direction



[101] = [110]

cubic

a=b=c



[101] ≠ [110]

tetragonal

- <123> Family of directions

أكثر من vector نفس الطول

نفس مقدار

  - [123], [213], [312], [132], [231], [321]

    only in a cubic crystal

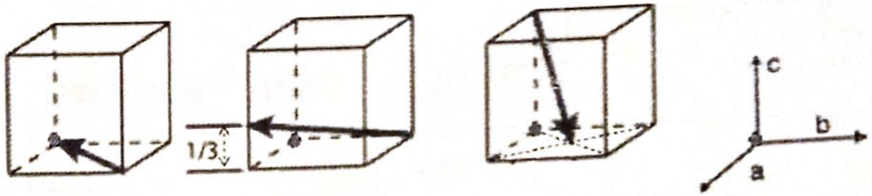
الـ Atom اللي بيمروا فيهم

*In the cubic system directions having the same indices regardless of **order** or **sign** are equivalent.*

في أي crystal system آخر لازم نحسب الطول حتى نعرف إذا بينتمي لنفس الـ family أو لا

Crystallographic direction, [uvw]

Example: (a,b,c) ….. [hkl]



$[\bar{1}\ \bar{1}\ 0]$ $[3\ \bar{3}\ 1]$ $[1\ 1\ \bar{2}]$

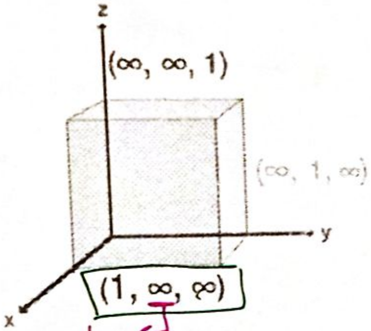
( )

Crystallographic Planes

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

- Algorithm

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



← موازي للمحور

← بنوخذ المطلوب عشان نتخلص من الـ ∞

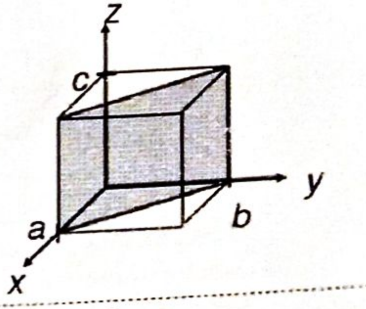
← إذا لقيت 2(0) صفرين ← بكون الـ plane مربع

← إذا لقيت (3) أرقام ← بكون الـ plane مثلث

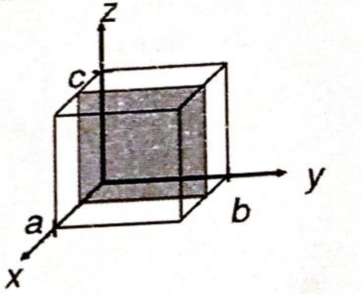
← إذا لقيت رقمين ← بكون plane مستطيل

Crystallographic Planes

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



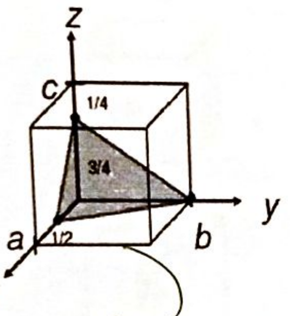
Example:		*a*	*b*	*c*
1.	Intercepts	1/2	∞	∞
2.	Reciprocals	1/½	1/∞	1/∞
		2	0	0
3.	Reduction	2	0	0
4.	Miller Indices	(200)		



Crystallographic Planes

Example:

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



مثلث ← 3 أرقام

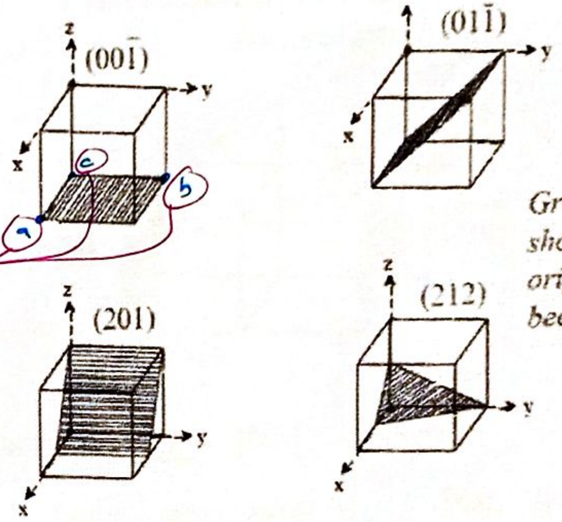
قاعدة Miller لل Planes اللي عل ال Origine :.

نحرك ال origine لفوق لتحت أو يمين شمال أو جوا برا ← لتوضيح صورة ال plane

← أكثر نقطة يعرفها Planes هي اللي بنحركها C

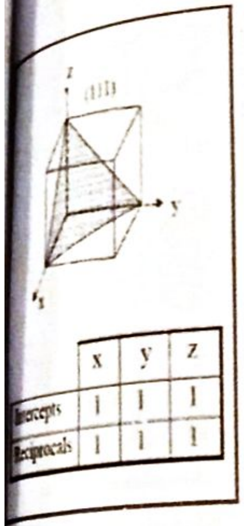
مهم جداً

Crystallographic planes



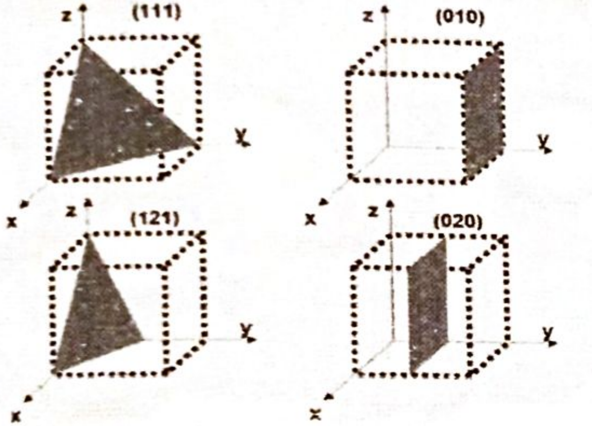
Green circles show where the origins have been placed.

Crystallographic planes



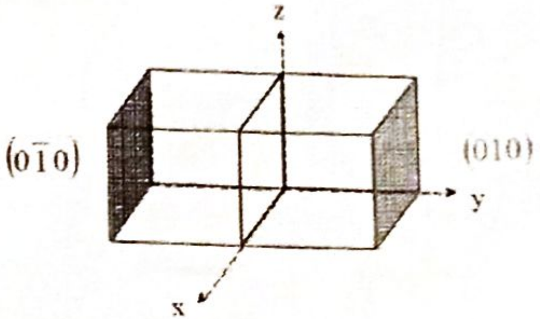
	x	y	z
Intercepts	1	1	1
Reciprocals	1	1	1

Crystallographic Planes: Miller Indices (hkl)



Crystallographic planes

Planes and their negatives are equivalent



Family of Planes $\{hkl\}$

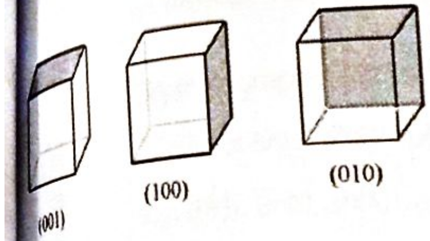
Ex: $\{100\} = (100), (010), (001), (\bar{1}00), (0\bar{1}0), (00\bar{1})$

Area نفس ال

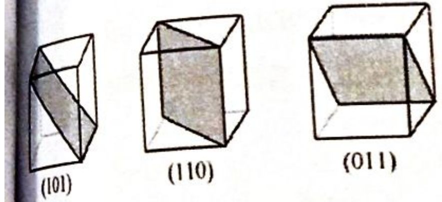
إذا منقلبة الأرقام ← نفس ال family

{ This all true for cubic Only }

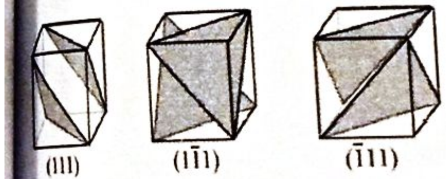
Crystallographic planes



In the cubic lattice, (100) is equivalent to five other planes, (010), (001), (100), (010), (001)

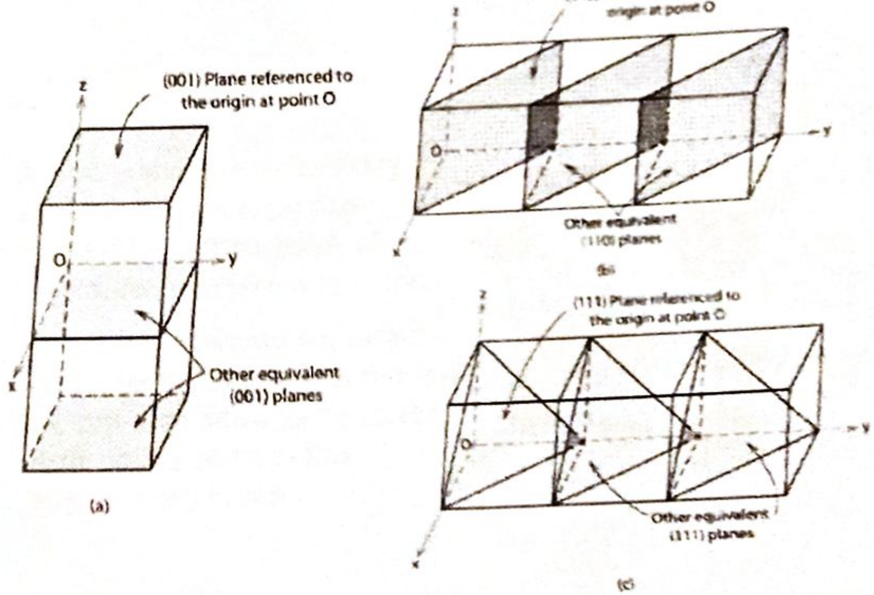


Equivalent plans



Equivalent plans

Crystallographic Planes



Adaplod from Fig. 3.9, *Callister 7e.*

Miller indices for planes

- (hkl) Crystallographic plane
- {hkl} Family of crystallographic planes { }
  e.g. (hkl), (lhk), (hlk).....etc
- In the *cubic* system planes having the same indices regardless of ***order*** or ***sign*** are equivalent.

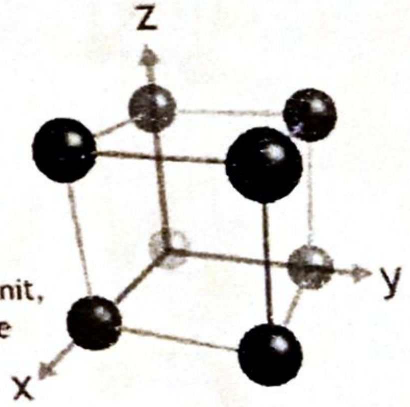
(001) (100) (010)

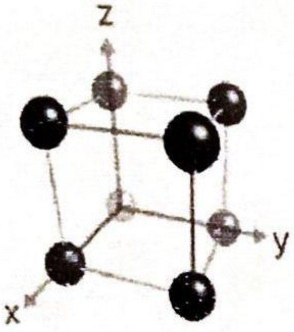
(hkl) **(lhk)** **(hlk)...etc.**

How to draw a lattice plane

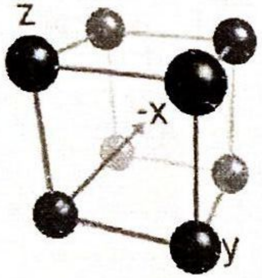
Just as you do when indexing a plane, it is necessary to choose the correct point of reference from which to work.

Taking the conventional origin at the far bottom left of the unit, we can then move along to the next lattice point in the x, y, or z directions.

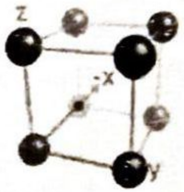




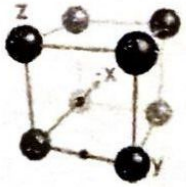
If you have a negative h index, move the point of reference along the x-axis to the other side of the unit cell, so that you can then go back in the negative x direction to find your intercept. Do the same for negative k and l indices.



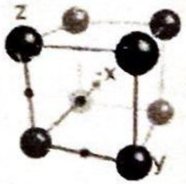
To draw the ($\bar{1}22$) plane, go back to -a on the x-axis,



go along to b/2 on the y-axis,



and go up to c/2 on the z-axis.



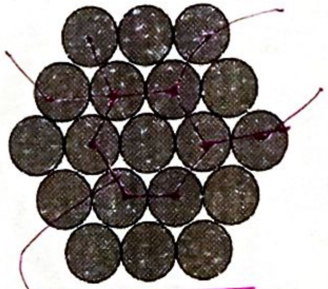
We can join these points to mark the trace of the plane on the unit cell surface, and then fill the plane.

ال structures الخاصة بالمعادن

Metallic Crystal Structures

- How can we stack metal atoms to minimize empty space?
- Two possible packing arrangement for spheres in a plane:

2-dimensions



vs.

square

Hexagonal packing

Square packing

This is the closest possible packing for uniform spheres

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

Metallic Crystal Structures

- Tend to be densely packed.
- Reasons for dense packing:

الرابطة الفلزية ← خاصة بالعنصر الواحد

- Typically, only one element is present, so all atomic radii are the same.

كل ال Atoms identical Atoms

ال Diameter و ال Radius نفسه لجميع الذرات

- Metallic bonding is not directional.
- Have the simplest crystal structures.

We will examine three such structures...

تشبق الذركي الوسط بسبب الرابطة الفلزية ← نفس عدد ال ة الموجود من حواليه كل Atom

الأشياء اللي بتميز فلي كل structure عن التاني simple أو center أو ... أو ...

الخصائص اللي لازم أميزها لكل structure:
① coordination #
② # of Atoms ~~الحجم~~
③ close paked direction
④ الحجم ← $\frac{4}{3}\pi R^3$ (# of Atoms)

← لازم نحفظ مثال ع الأقل على كل نوع من ال structure

Simple Cubic Structure (SC)

- Rare due to low packing density, only Po (Polonium) has this structure.

بتكون طولها 2R

- Close-packed directions are cube edges. → 2R
- Coordination # = 6 (# nearest neighbors)

كم Atom ملامسة لل Atom

عبارة عن جزء من 8 unit cells

ال unit cell

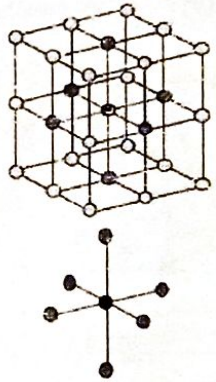
2R → Close packed direction

every Atom in the space is shared with 8 unit cellss

عنصر هيك تركيبة

بولونيوم

(Courtesy P.M. Anderson)



10^{23} Atom موجودة في ال space على شكل منتظم

Simple Cubic structure

* ال Atoms دائمًا تأتي على زوايا المكعب
* العنصر اللي هيك تركيبه البولونيوم
* ال unit cell كـ volume تكون Atom واحدة لأنه كل unit cell تأخذ $\frac{1}{8}$ من ال Atom وتحتوي

ال unit cell ← 8 ذرات ← $1 = 8 * \frac{1}{8}$

← حجم ال unit cell ← $\frac{4}{3}\pi R^3 * 1$

Body Centered Cubic Structure (BCC)

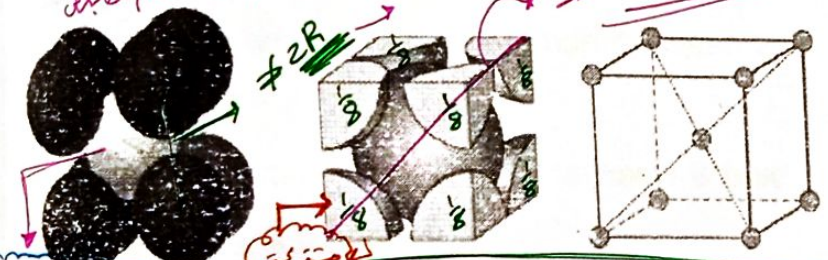
- Atoms touch each other along cube diagonals.

Note. All atoms are identical; the center atom is shaded differently only for ease of viewing.

ex: Cr (chromium), W (Tungsten), Fe (α), (Ta) Tantalum, (Mo) Molybdenum

لأنه الذرات اللي بالنص بيحتكوا مع بعض

4R close pake direction



غير مشتركة بين أجزاء unit cell

2 atoms/unit cell: 1 center + 8 corners x 1/8 Volume

- Coordination # = 8

(Courtesy P.M. Anderson) Adapted from Fig. 3.2, *Callister 7e*.

Body center cubic

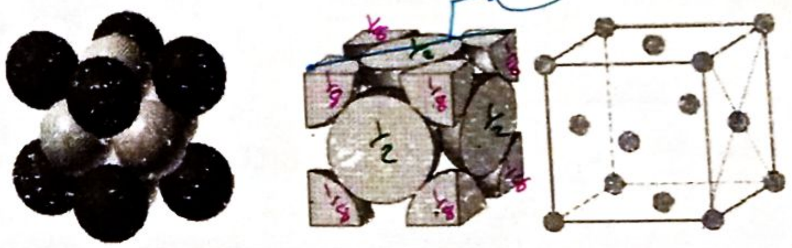
coordination # = 8

Face Centered Cubic Structure (FCC)

- Atoms touch each other along face diagonals.
  - --Note: All atoms are identical; the face-centered atoms are shaded differently only for ease of viewing.

ex: Al (Aluminium), Cu (Copper), Au (Gold), Pb (Lead), Ni (Nickel), Pt (Platinum), Ag (Silver)

4R



4 atoms/unit cell: 6 face x 1/2 + 8 corners x 1/8 *

(Courtesy P.M. Anderson) Adapted from Fig. 3.1, *Callister 7e*.

- Coordination # = 12 *

# of Atoms 4

face diagonal

Crystal structure

To find the number of the atoms are contained within the 3-Dimensional unit cell, the following rules are applied:

- Eight unit cells meet at the corner of a unit cell
- Each face of the unit cell is common between 2 cells
- The corner atom will be shared between 8 unit cells that meet at that point
- The atom positioned in the cell face will be shared between 2 cells.

شرط ثبات الكتلة

كلما زاد ـ زادت الكثافة

* دائمًا لإيجاد العلاقة بين R و a نستخدم ال closed packed direction

* حجم الذرات بالنسبة للحجم الكلي

حجم الكرة * عدد الذرات

المحسوبة سابقًا

$\frac{1}{8} * 8$

simple cubic

Atomic Packing Factor (APF)

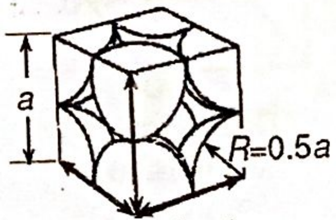
$$APF = \frac{\text{Volume of atoms in unit cell*}}{\text{Volume of unit cell}}$$

*assume hard spheres

الحجم للذرات بدون الفراغات

حجم ال unit cell شامل الفراغات

- APF for a **simple cubic structure** = 0.52



close-packed directions

contains 8 x 1/8 = 1

1 atom/unit cell

Adapted from Fig. 3.23, *Callister 7e.*

$$APF = \frac{\overset{\frac{\text{atoms}}{\text{unit cell}}}{1}\ \overset{\frac{\text{volume}}{\text{atom}}}{\frac{4}{3}\pi(0.5a)^3}}{\underset{\frac{\text{volume}}{\text{unit cell}}}{a^3}}$$

$$APF = \frac{1*\left(\frac{4}{3}\pi\left(\frac{a}{2}\right)^3\right)}{a^3} = \frac{4}{3}\pi\frac{a^3}{8}\frac{1}{a^3}$$

$$APF = \frac{\pi}{6} = 0.52$$

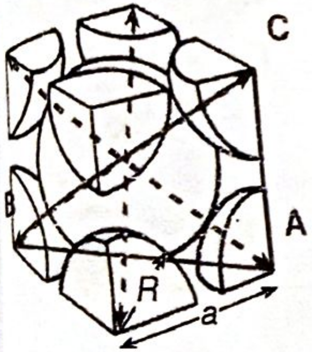
* الفائدة من هذه الفراغات (0.48) لخلط المواد معًا لمعرفة ال optimal للـ Alloy لمعرفة كم نسبة المادة المضافة

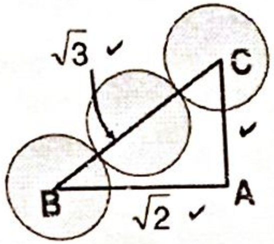
Atomic Packing Factor: BCC

$$APF = \frac{\text{Volume of atoms in unit cell*}}{\text{Volume of unit cell}}$$

*assume hard spheres

- To find volume of an atom, we need to find r = f(a); where r: atom radius, a: lattice constant





Close-packed directions:
Length= $4R = \sqrt{3}\,a$

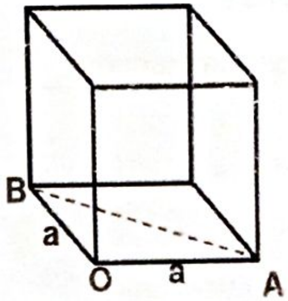
$$Apf = \frac{\frac{4}{3}\pi R^3 * \textcircled{2}}{a^3} \rightarrow$$ # of Atoms

$$= \frac{\frac{4}{3}\pi \cancel{R^3} * 2}{\frac{64 \cancel{R^3}}{(\sqrt{3})^3}} = 0.68$$

$$(4R)^2 = a^2 + (\sqrt{2}a)^2$$

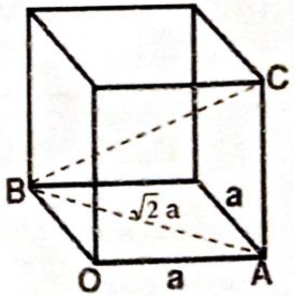
$$16R^2 = 3a^2 \rightarrow \boxed{a = \frac{4R}{\sqrt{3}}}$$

Atomic Packing Factor: BCC



Triangle OAB

$$AB^2 = OA^2 + OB^2$$
$$AB^2 = a^2 + a^2$$
$$AB^2 = 2a^2$$
$$AB = \sqrt{2}a$$



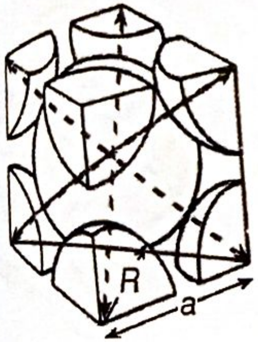
Triangle ABC

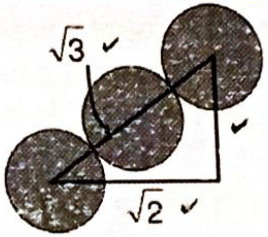
$$BC^2 = AB^2 + AC^2$$
$$BC^2 = \left(\sqrt{2}a\right)^2 + a^2$$
$$BC^2 = 2a^2 + a^2 = 3a^2$$
$$BC = \sqrt{3}a$$

الفراغ = 0.32

Atomic Packing Factor: BCC

- APF for a body-centered cubic structure = $\boxed{0.68}$





Close-packed directions:
length = $4R = \sqrt{3}\,a$

$$\frac{\text{atoms}}{\text{unit cell}} \rightarrow \quad \mathrm{APF} = \frac{2\ \frac{4}{3}\pi\,(\sqrt{3}a/4)^3}{a^3} \quad \begin{matrix} \leftarrow \frac{\text{volume}}{\text{atom}} \\ \leftarrow \frac{\text{volume}}{\text{unit cell}} \end{matrix}$$

Adapted from Fig. 3.2(a), *Callister 7e.*

Atomic Packing Factor: BCC

$$\mathrm{APF} = \frac{\text{Volume of atoms in unit cell*}}{\text{Volume of unit cell}}$$

*assume hard spheres

$$APF = \frac{2\left(\frac{4}{3}\pi r^3\right)}{a^3}, \quad r = \frac{\sqrt{3}}{4}a$$

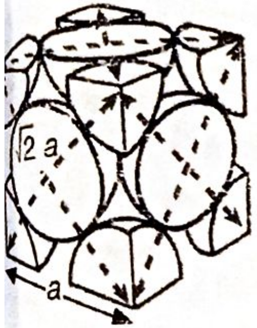
$$APF = \frac{2\left(\frac{4}{3}\pi\left(\frac{\sqrt{3}}{4}a\right)^3\right)}{a^3}$$

$$APF = 2\,\frac{4}{3}\pi\,\frac{3\sqrt{3}a^3}{64}$$

$$APF = \frac{\pi\sqrt{3}}{8}$$

$$\boxed{APF = 0.68}$$

Atomic Packing Factor: FCC



The atoms touch one another across a face-diagonal, the length of this is 4R

$$a^2 + a^2 = (4R)^2$$

$$2a^2 = 16R^2$$

$$a = 2\sqrt{2}R$$

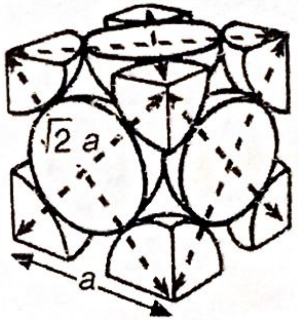
Volume of the unit cell $V_c = a^3 = \left(2\sqrt{2}R\right)^3 = 16\sqrt{2}R^3$

Adapted from Fig. 3.1(a), *Callister 7e.*

Atomic Packing Factor: FCC

- APF for a face-centered cubic structure = $\boxed{0.74}$

maximum achievable APF



Close-packed directions:
length = 4*R* = √2 *a*

Unit cell contains:
6 x 1/2 + 8 x 1/8
= 4 atoms/unit cell

$$\mathrm{APF} = \frac{\frac{\text{atoms}}{\text{unit cell}} \rightarrow 4\ \frac{4}{3}\pi(\sqrt{2}a/4)^3 \leftarrow \frac{\text{volume}}{\text{atom}}}{a^3 \leftarrow \frac{\text{volume}}{\text{unit cell}}}$$

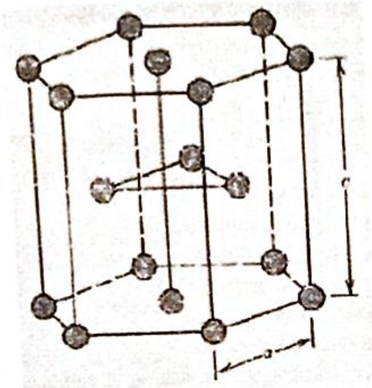
Adapted from Fig. 3.1(a), *Callister 7e.*

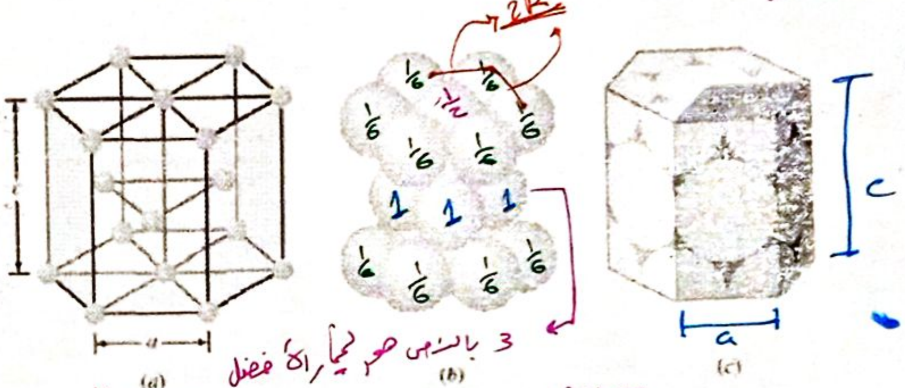
in the ideal cube
All the atoms are
the same

$$\boxed{\frac{c}{a} = 1.633}$$

Hexagonal Closed Packed (HCP)

- Two lattice parameters: a and c, representing the basal and height parameters respectively.
- The ideal c/a ratio is 1.633.
- Number of atoms per unit cell (N) = 6 atoms.
- Atomic packing factor is 0.74
- Coordination number (CN) = 12.





3 بالنص حتى يصير الأفضل

⇐ لتقليل المسافات بين الذرات وليصير بشكل منتظم

Figure 3.6
HCP unit cells: (a) atomic-site unit cell, (b) hard-sphere unit cell, and (c) isolated unit cell.
[(b) and (c) After F. M. Miller, "Chemistry: Structure and Dynamics," McGraw-Hill, 1984, p. 296.]

N = # corner atoms + # central atoms + # face center atoms

$$N = 2\left(6x\frac{1}{6}\right) + 3x1 + \left(2x\frac{1}{2}\right)$$

N = 6 atoms / unit cell

# of Atoms → $\frac{1}{6} * 12 + 3 + \frac{1}{2} * 2$

⇒ $\boxed{\text{\# of Atoms} = 6}$

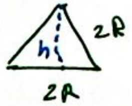
Coordination # → $\boxed{12}$

close packed direction → 2R

$$Apf = \frac{\frac{4}{3}\pi R^3 (6)}{(6 * \frac{1}{2} a h)(c)}$$

$$= \frac{\frac{4}{3}\pi \cancel{R^3}(6)}{3(2\cancel{R})(\sqrt{3})\cancel{R}(1.633)(\cancel{2R})} = 0.74$$

a = 2R



→ $\boxed{h = \sqrt{3} R}$

---

from the ratio

c = 1.633 a

c = (1.633)(2R)

Hexagonal Closed Packed (HCP)

Show how to calculate the APF for the HCP?

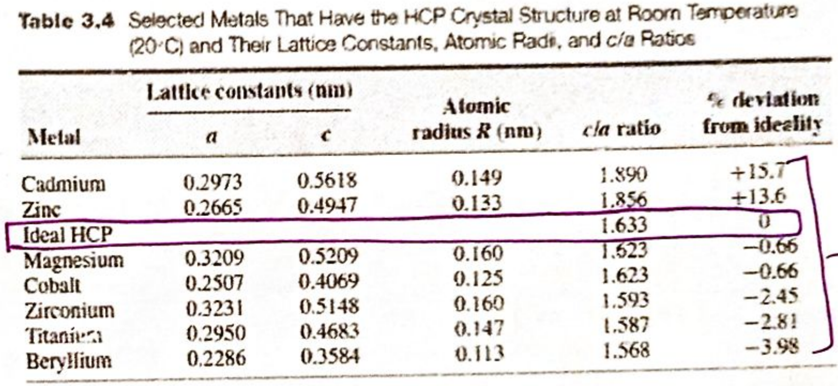


Table 3.4 Selected Metals That Have the HCP Crystal Structure at Room Temperature (20°C) and Their Lattice Constants, Atomic Radii, and *c/a* Ratios

Metal	Lattice constants (nm)		Atomic radius *R* (nm)	*c/a* ratio	% deviation from ideality
	a	*c*			
Cadmium	0.2973	0.5618	0.149	1.890	+15.7
Zinc	0.2665	0.4947	0.133	1.856	+13.6
Ideal HCP				1.633	0
Magnesium	0.3209	0.5209	0.160	1.623	−0.66
Cobalt	0.2507	0.4069	0.125	1.623	−0.66
Zirconium	0.3231	0.5148	0.160	1.593	−2.45
Titanium	0.2950	0.4683	0.147	1.587	−2.81
Beryllium	0.2286	0.3584	0.113	1.568	−3.98

سبب الخلل هو ال error الموجود في الأجهزة والعملية المستخدمة في قياس هذه الحالات

+ الذبذبة ال Vibration

+ وجود بعض الذرات الأخرى

+

Crystal structure

Atomic Radii and Crystal Structures for 16 Metals

tal	Crystal Structure[a]	Atomic Radius[b] (nm)	Metal	Crystal Structure	Atomic Radius (nm)
luminum	FCC	0.1431	Molybdenum	BCC	0.1363
Cadmium	HCP	0.1490	Nickel	FCC	0.1246
Chromium	BCC	0.1249	Platinum	FCC	0.1387
Cobalt	HCP	0.1253	Silver	FCC	0.1445
Copper	FCC	0.1278	Tantalum	BCC	0.1430
Gold	FCC	0.1442	Titanium (α)	HCP	0.1445
Iron (α)	BCC	0.1241	Tungsten	BCC	0.1371
Lead	FCC	0.1750	Zinc	HCP	0.1332

[a] FCC = face-centered cubic; HCP = hexagonal close-packed; BCC = body-centered cubic.

[b] A nanometer (nm) equals 10^{-9} m; to convert from nanometers to angstrom units (Å), multiply the nanometer value by 10.

ـ الفرق ما بين القيم المحسوبة والحقيقية يرجع لـ:-

① التشققات في المادة

② عدم التراص 100% للـ unit cell

تشكيل الـ structure على شكل planes

Crystal structure

close packed direction	Unit cell	No. atoms / unit cell	Coordination number	A.P.F.	Stacking sequence	r = f(a)
cube edges	Simple cubic , SC	1	6	0.52		0.5a =R
Body Diagonal	Body centered cubic, BCC	2	8	0.68		$\frac{\sqrt{3}}{4}a$ =R
face diagonal	Face centered cubic , FCC	4	12	0.74	ABCABC..	$\frac{\sqrt{2}}{4}a$ =R
edges	Hex. closed packed , HCP	6	12	0.74	ABAB....	

*The 3-D build up of the crystal is formed by stacking a series of the (110) – the most dense packed plane