THE UNIVERSITY OF ZAMBIA
SCHOOL OF ENGINEERING
DEPARTMENT OF MECHANICAL ENGINEERING

MEC 2309 – PROPERTIES OF ENGINEERING MATERIALS I

LECTURE 2

ATOMIC STRUCTURE AND INTER-ATOMIC BONDING

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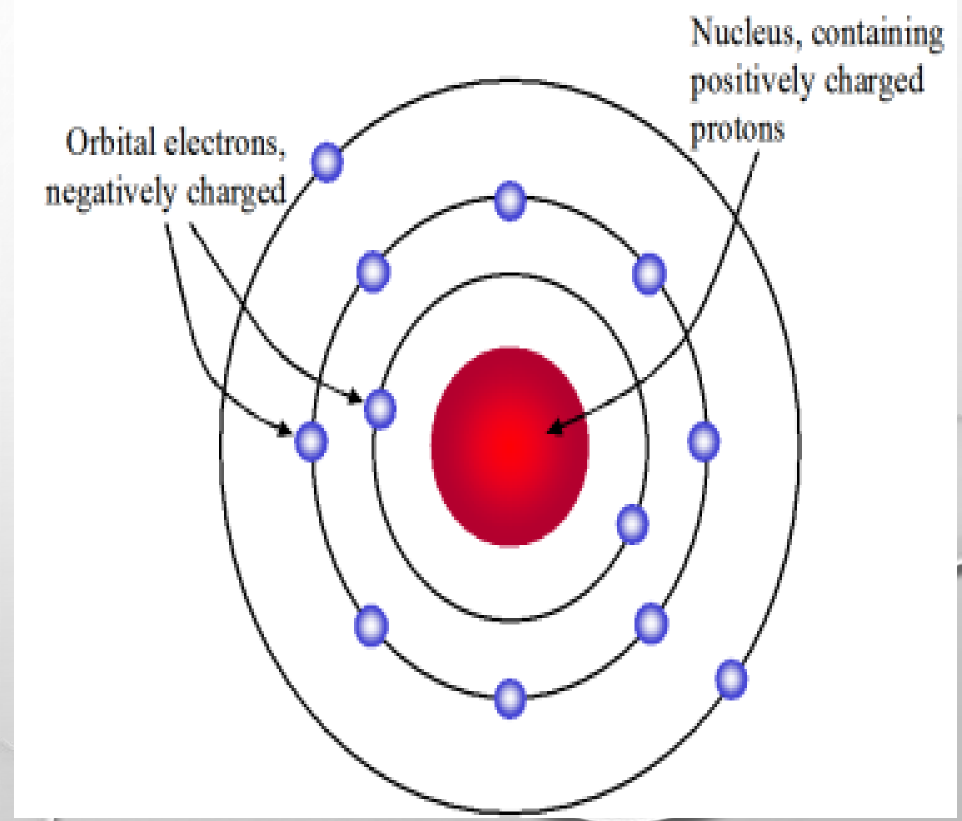
ATOMIC STRUCTURE OF MATERIALS

- The properties of solid materials significantly depend on **geometrical atomic arrangements**, and also the **interactions** that exist among constituent atoms or molecules.
- Properties depend on how atoms are **arranged** and **bonded** one to another.
- This lecture considers several fundamental and important concepts—namely, atomic structure, electron configurations in atoms and the periodic table, and the various types of primary and secondary interatomic bonds that hold together the atoms that compose a solid.

ATOMIC STRUCTURE OF MATERIALS

- All materials are made of atoms
- Each atom consists of a very small nucleus composed of protons and neutrons, which is encircled by moving electrons.
- Both electrons and protons are electrically charged.
- The charge magnitude being $\mathbf{1.602 \times 10^{-19} C}$, which is negative (-) in sign for electrons and positive (+) for protons; neutrons are electrically neutral.



ATOMIC STRUCTURE OF MATERIALS

- Number of protons in the nucleus = **atomic number (Z).** Ranges in integral units from 1 for hydrogen to 92 for uranium, the highest of the naturally occurring elements (118 in total including the man made elements.
- The **atomic mass (A) =** the sum of the masses of protons and neutrons within the nucleus of an atom.
- The number of protons is the same for all atoms of a given element, although the number of **neutrons (N)** may vary giving rise to isotopes.
- The **atomic weight** of an element corresponds to the weighted average of the atomic masses of the atom's naturally occurring isotopes.
- The atomic weight of an element or the molecular weight of a compound may be specified on the basis of mass per mole of material.
- In one mole of a substance there are $\mathbf{6.022 \times 10^{23}}$ **(Avogadro's number)** atoms or molecules.
- For example, the atomic weight of iron is 55.85 g/mol.

ATOMIC STRUCTURE OF MATERIALS

- Electrons exist in separate orbitals or energy states surrounding the nucleus.

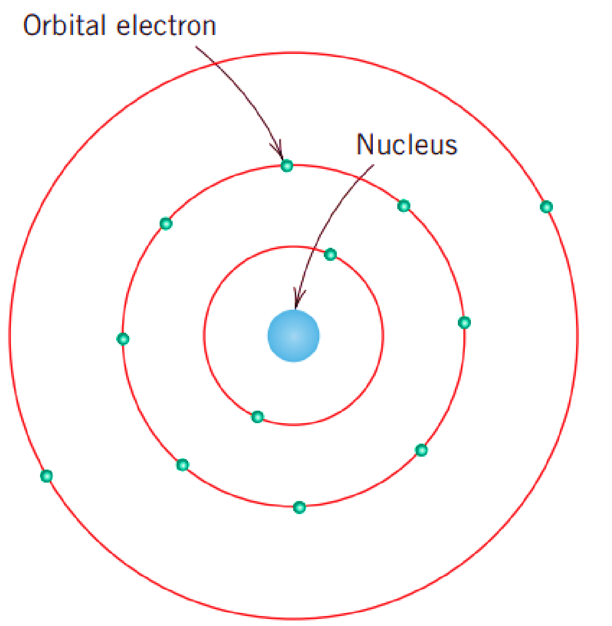


Table 1: **The Number of Available Electron States in Some of the Electron Shells and Subshells**

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

ATOMIC STRUCTURE OF MATERIALS

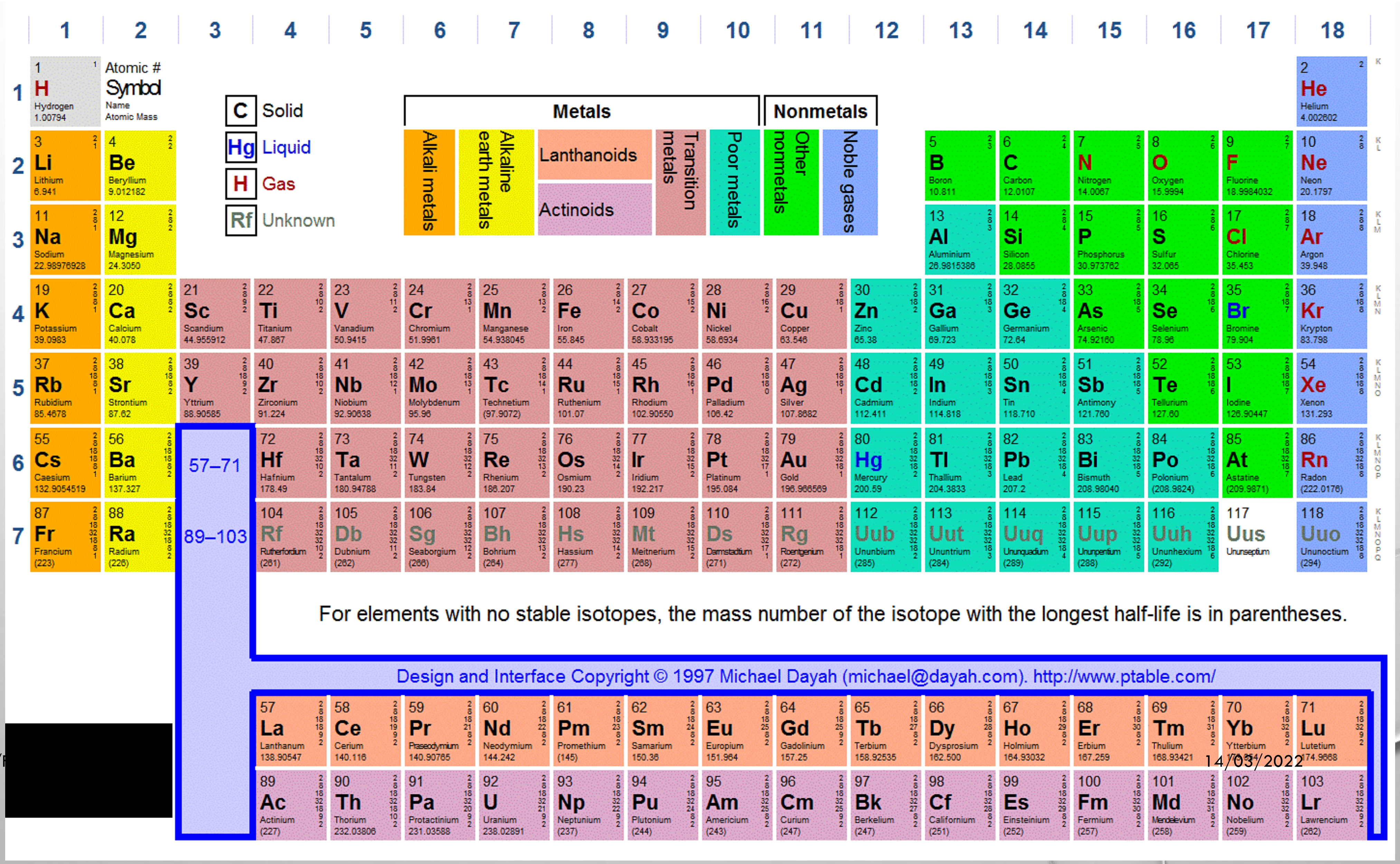
- The first inner shell (known as the K shell) has two positions for electrons, the next shell (the L shell) has 8.
- Therefore hydrogen (whose atomic number is 1) will only have one electron in the first shell, or 1k electron.
- Helium will have 2 k electrons, lithium will have 2 k electrons and 1 l electron, beryllium will have 2 k electrons and 2 l electrons, boron will have 2 k electrons and 3 l electrons, and so forth.
- **This periodic filling of the electron shells results in a periodic variation of properties of atoms as you increase in atomic number. This is the basis of the periodic table.**

PERIODIC TABLE OF THE ELEMENTS

Group→ ↓Period	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba		72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra		104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Fl	115 Uup	116 Lv	117 Uus	118 Uuo

Lanthanides	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
Actinides	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

PERIODIC TABLE OF THE ELEMENTS



ATOMIC STRUCTURE OF MATERIALS

Bonding forces between any two or more atoms may be:

- Ionic, covalent or metallic bonding –termed **primary bonds** - strong, or
- Van der waals bonding – **secondary bonds** - weak.

The different properties of materials depend on the widely differing nature of these four bonds.

ATOMIC STRUCTURE OF MATERIALS

IONIC BOND

- Simplest type of bond

- From electrostatic or coulombic forces (of attraction) between +ve and –ve ions in solid crystals

- This bond is non-directional leading to freedom in the way they pack

ATOMIC STRUCTURE OF MATERIALS

IONIC BOND

Ionic bonds are strong and stiff. As a result they generally give a material with:

- High strength
- High elastic modulus
- High melting point
- Poor electrical conductivity

Some examples of ionic bonding are:

- Magnesia (mgo)
- Alumina (al2o3)
- Cement

ATOMIC STRUCTURE OF MATERIALS

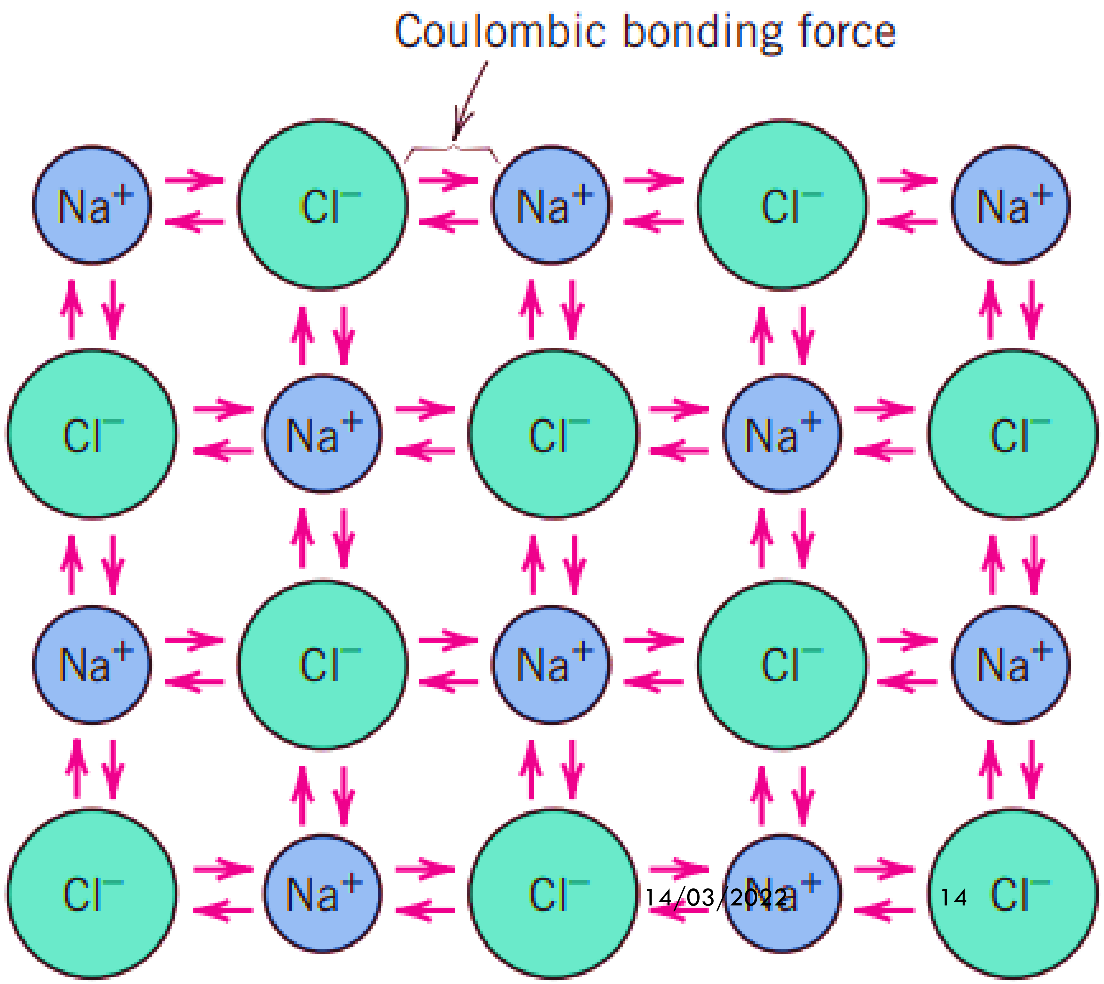
IONIC BOND

- In ionic bonds, however, ions can separate easily in a dielectric media, like water.
- Thus most ionic crystals are hygroscopic, and easily dissolve in water.
- Ionic crystals are transparent as single crystals and are used mainly for lenses in scientific instruments.

IONIC BOND

2D View of NaCl Structure

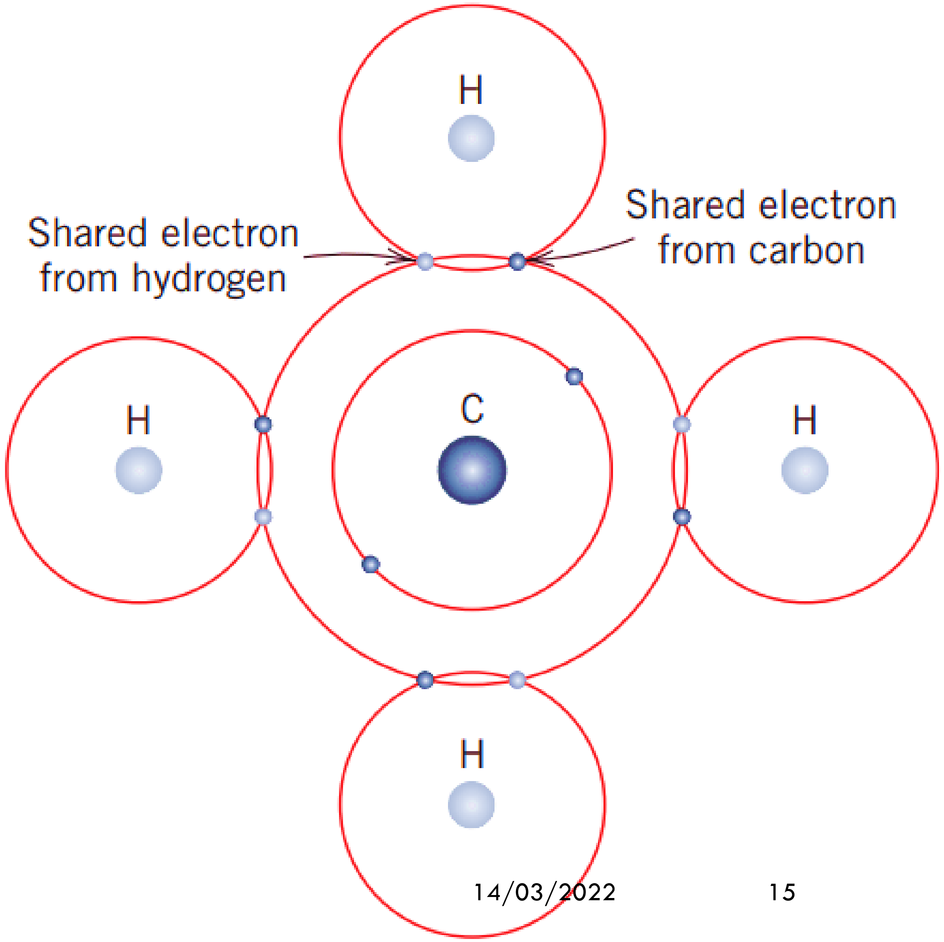
- Example: Sodium Chloride (Common Salt, NaCl)
- Na^+ ions are surrounded by six Cl^- and
- Similarly, a Cl^- ion is surrounded by six Na^+ ions.



ATOMIC STRUCTURE OF MATERIALS

COVALENT BOND

- Results from two atoms sharing electrons.
- For each covalent bond, two electrons are involved.
- Covalent bonds are localised and directional in nature.
- This directionality dictates the atomic packing



ATOMIC STRUCTURE OF MATERIALS

COVALENT BOND

Covalent bonds can be very stiff and generally give a material with:

- Very high elastic modulus
- High (inherent) strength – though at times brittle
- High melting point
- Low electrical conductivity
- Covalent bonding is the dominant bonding found in silicate ceramics and glasses. It also occurs in the backbone of polymer chains and in the cross-links in thermosetting polymers.

ATOMIC STRUCTURE OF MATERIALS

COVALENT BOND

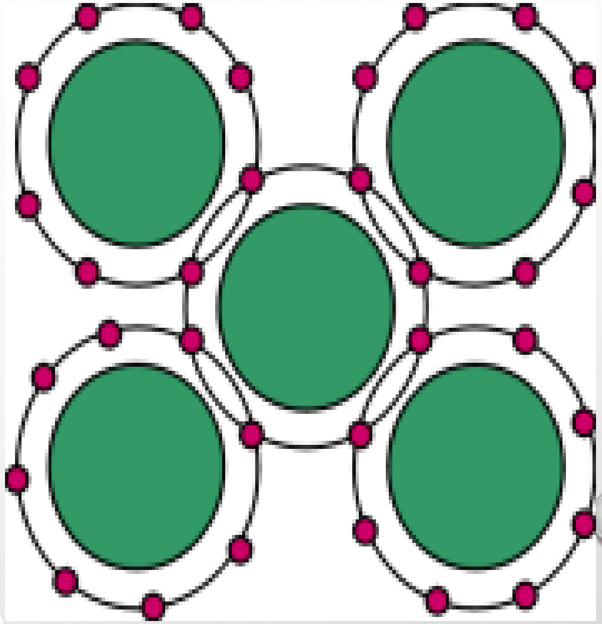
Examples:

1. **Diamond** :

- Hardest material in nature
- Consists entirely of covalent bonds.
- The directional nature of the bond leads to a ***tetrahedral*** arrangement – bonds directed towards the four corners of the tetrahedron (= solid figure with four triangular surfaces).

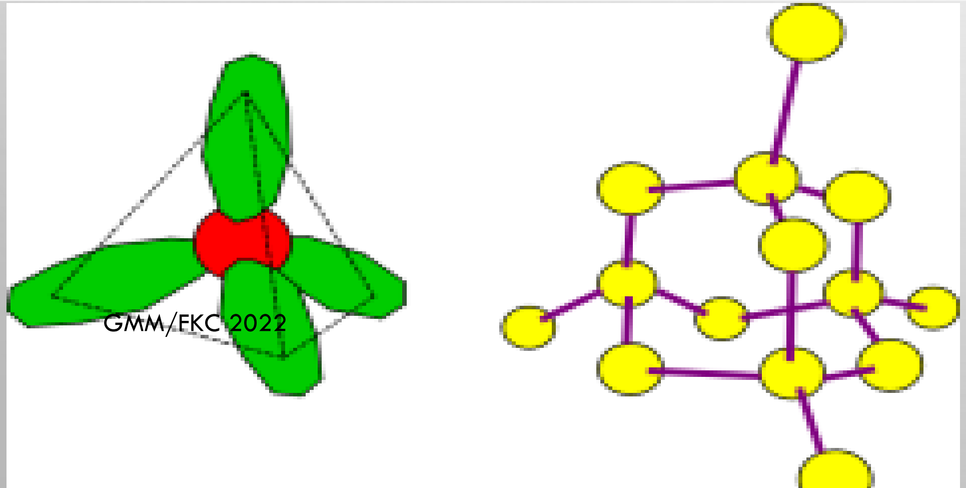
ATOMIC STRUCTURE OF MATERIALS

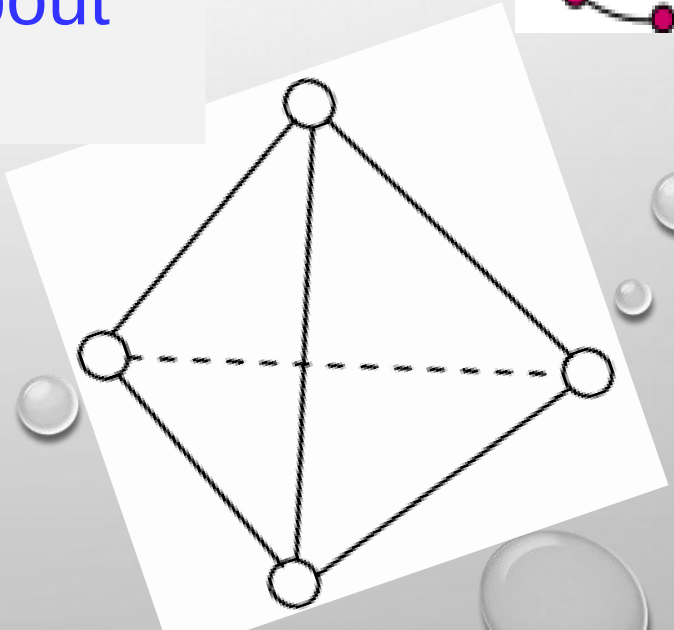
COVALENT BOND



CARBON TETRAHEDRON

- Due to the strong C-C bonds, diamond is ***very hard*** and is also ***stable up to very high temperatures*** (up to about 3,000^{o}C).





ATOMIC STRUCTURE OF MATERIALS

COVALENT BOND

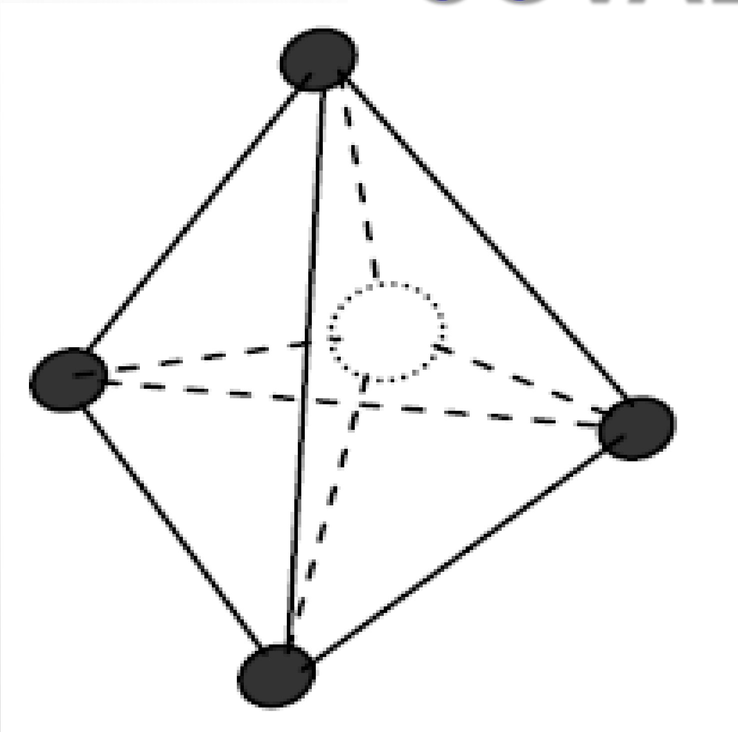
2. **Silica (SiO)** - existing in two forms:

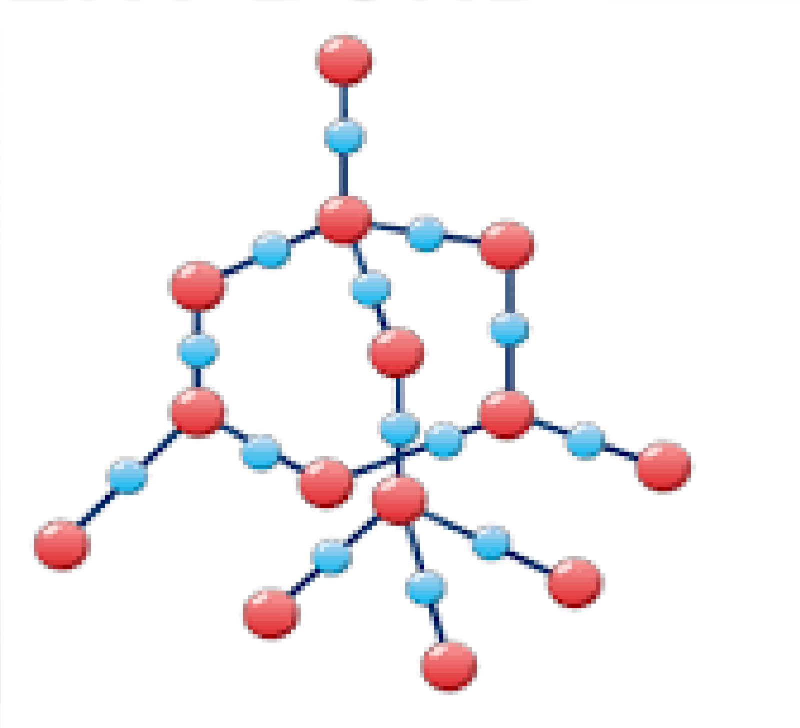
- Crystalline silica, called ***quartz***
- Amorphous silica, called ***fused silica*** or ***fused quartz***.

- A ***si*** atom is situated inside the tetrahedron with four ***o*** atoms at the four corners.
- In the solid, tetrahedrons or ***tetrahydra*** are joined at the corners.
- In amorphous silica, tetraheda are in zig-zag or random manner (although joined at the corners).

ATOMIC STRUCTURE OF MATERIALS

COVALENT BOND





- Oxygen Atoms
- Silicon Atoms

- Because of the covalent nature of the si-o bonds, silica is a very strong solid with a melting point of about 1710ºc.

ATOMIC STRUCTURE OF MATERIALS

COVALENT BOND

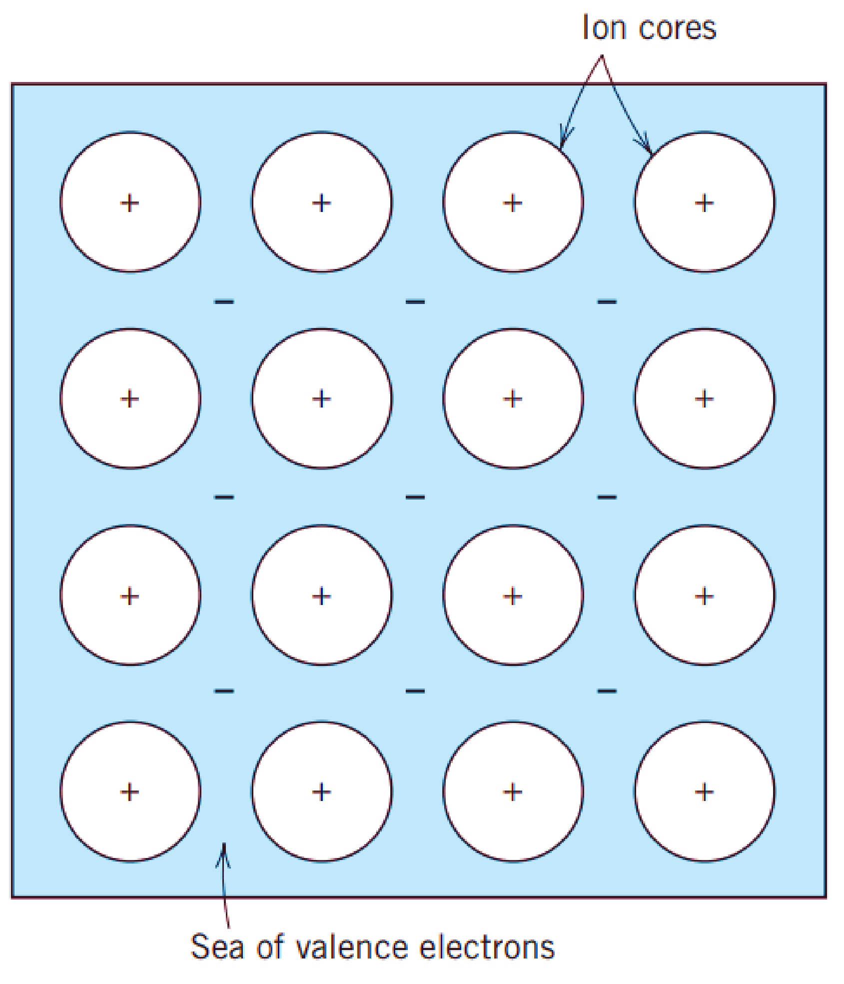
Uses of some covalently bonded materials:

- **Quartz crystals** – as piezoelectric crystals for oscillators, timers, quartz watches, etc.
- **Amorphous silica** – basic skeleton for the structure of glass. Ions such as Na^+ and K^+ occupy the voids between the tetrahedra in glass.

ATOMIC STRUCTURE OF MATERIALS

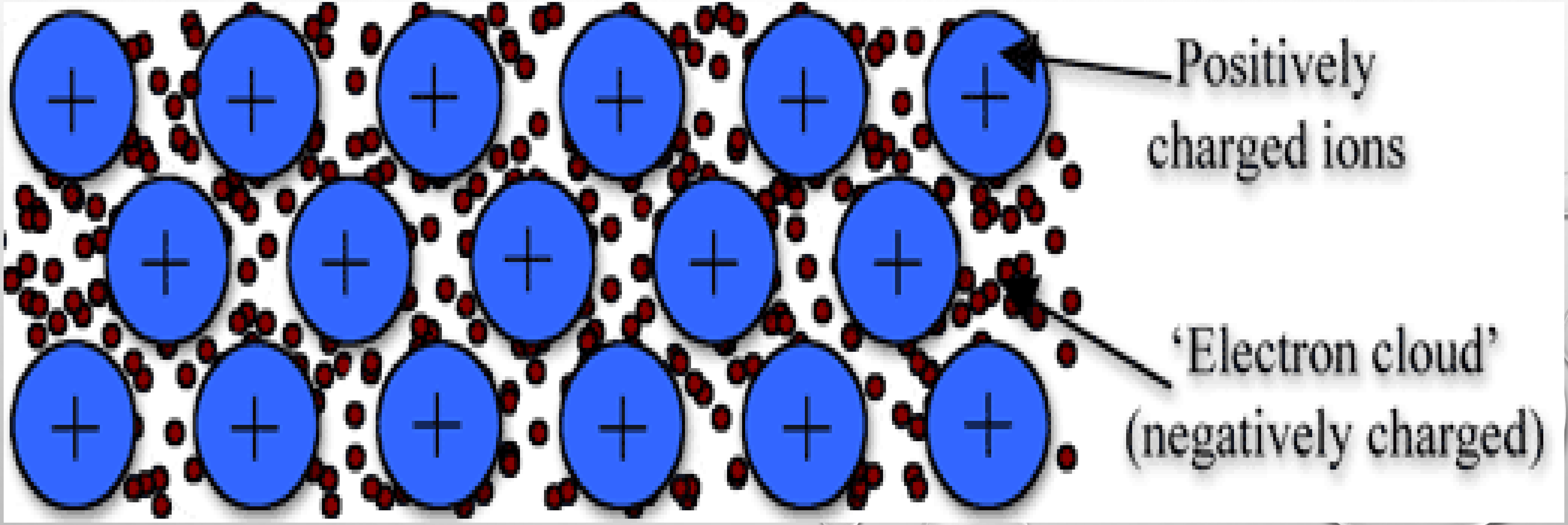
METALLIC BOND

- Present in almost all metals
- Characterised by delocalised nature of the bond
- Metallic crystals consist of positively charged ions with delocalised valence or “conduction” electrons moving about freely in the crystal.
- The electrons are “surrendered” to a common pool and become shared by all the atoms in the solid metal.



ATOMIC STRUCTURE OF MATERIALS

METALLIC BOND



ATOMIC STRUCTURE OF MATERIALS

METALLIC BOND

- Bonds are non-directional
- Atoms tend to form crystal structures which resemble close packing of spheres with the conduction electrons forming an electron gas or cloud
- Metals tend to be very good conductors of electricity and heat
- Metallic ions also move freely with respect to each other leading to high plasticity of metals

ATOMIC STRUCTURE OF MATERIALS

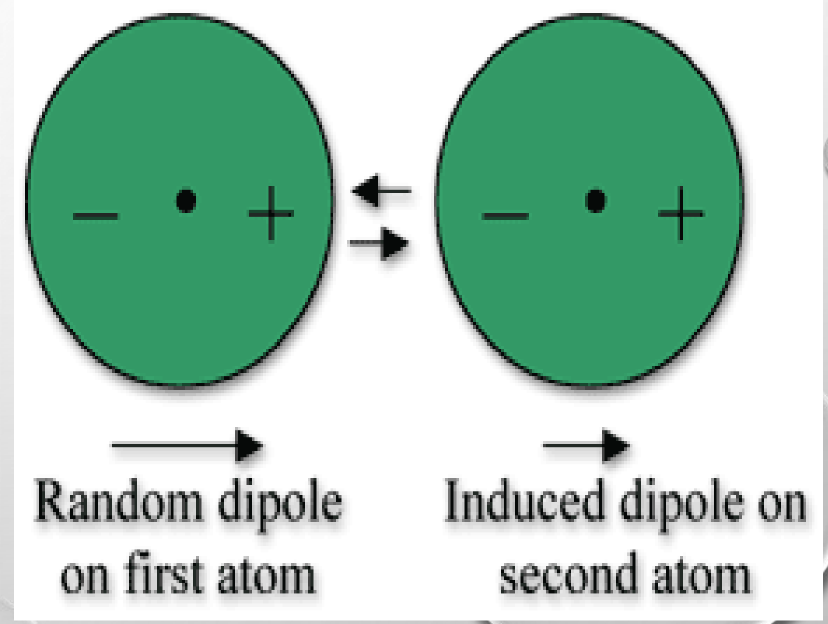
SECONDARY BONDING – VAN DER VAALS BOND

- Weak bond
- Secondary bonds are not bonds with a valence electron being shared or donated.
- They are usually formed when an uneven charge distribution occurs, creating what is known as a dipole (the total charge is zero, but there is slightly more positive or negative charge on one end of the atom than on the other).
- Attraction = polarisation (separation of the centres of +ve and –ve charges in an electrically neutral atom or molecule as it is brought close to its neighbours) of the electric charges in atoms.

ATOMIC STRUCTURE OF MATERIALS

SECONDARY BONDING – VAN DER VAALS BOND

- Common between covalently bonded chains of atoms in polymers, and the attraction between gas molecules
- **E.G.** Hydrogen bonds in water and some organic materials: 0ºc < m. P. < 400ºc.



ATOMIC STRUCTURE OF MATERIALS

In many materials, a combination of bonding types is involved.

- In graphite, sheets of carbon atoms are covalently bonded within the sheet, with sheets held by van der waals bonds. Thus graphite is soft as one layer of atoms can slip over another layer making it suitable as a lubricant for bushings.

- Other materials with sheet structures are mica and talc.

- Materials like polymers also consist of atoms covalently bonded in chains held together by weak van der waals bonds.

ATOMIC STRUCTURE OF MATERIALS

- Atoms and molecules are the building blocks of more macroscopic structure of matter

- When materials solidify from the molten state, they tend to close ranks and pack tightly, arranging themselves into one of two structures:

✓ **Crystalline**

✓ **Non-crystalline and/or Amorphous**

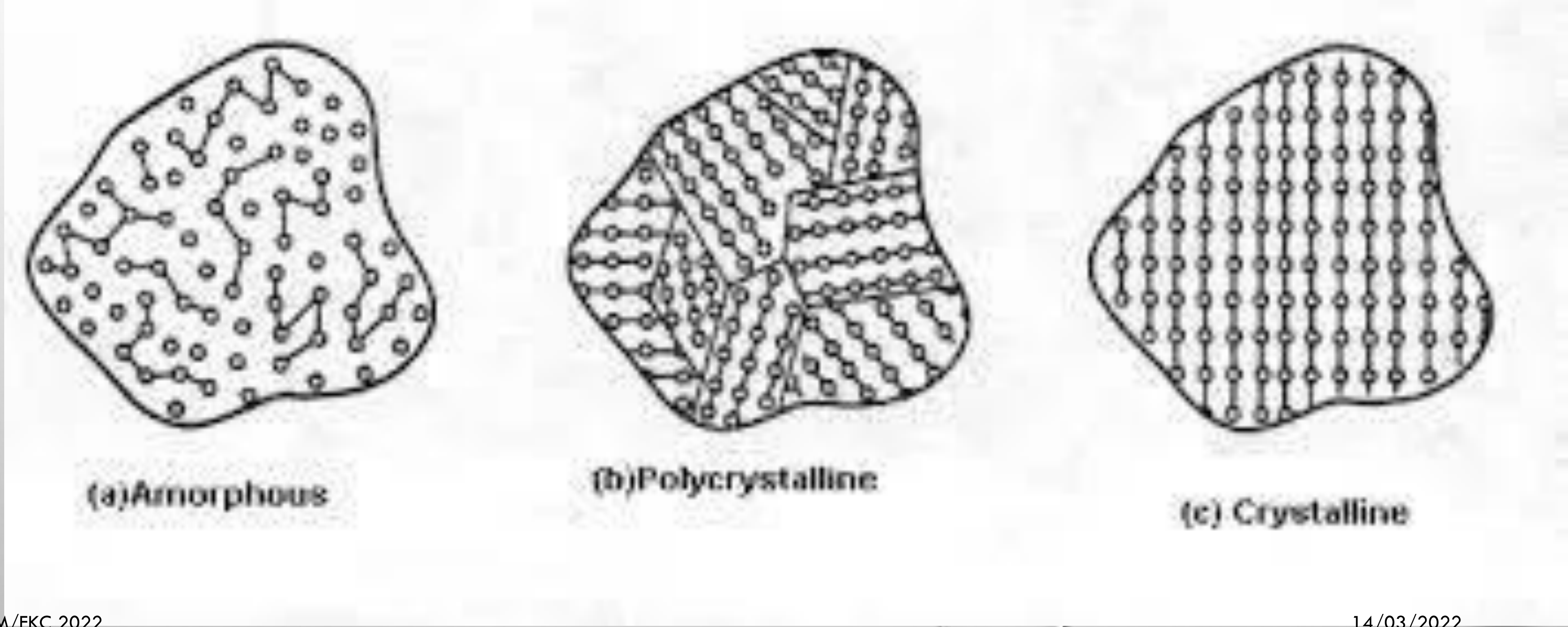
ATOMIC STRUCTURE OF MATERIALS

- A **crystalline** material is one in which the atoms are situated in a repeating or periodic array over large atomic distances; that is, long-range order exists, such that upon solidification, the atoms will position themselves in a repetitive three dimensional pattern, in which each atom is bonded to its nearest-neighbor atoms.
- All **metals**, **many ceramic materials**, and **certain polymers** form crystalline structures under normal solidification conditions.
- .

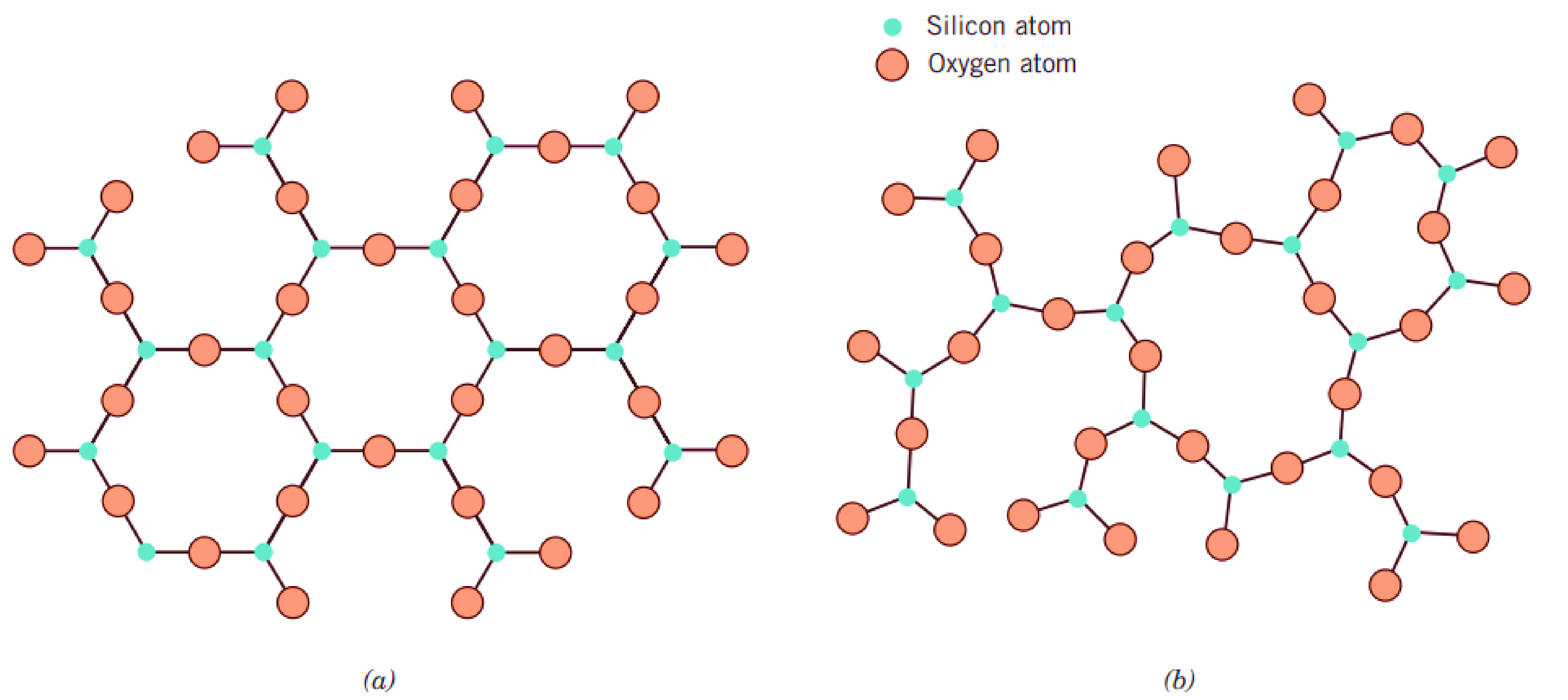
ATOMIC STRUCTURE OF MATERIALS

- Non-crystalline solids lack a systematic and regular arrangement of atoms over relatively large atomic distances.
- Sometimes such materials are also called amorphous (meaning literally “without form”), or supercooled liquids, as their atomic structure resembles that of a liquid.
- Rapidly cooling through the freezing temperature favors the formation of a non-crystalline solid, because little time is allowed for the ordering process

ATOMIC STRUCTURE OF MATERIALS



ATOMIC STRUCTURE OF MATERIALS

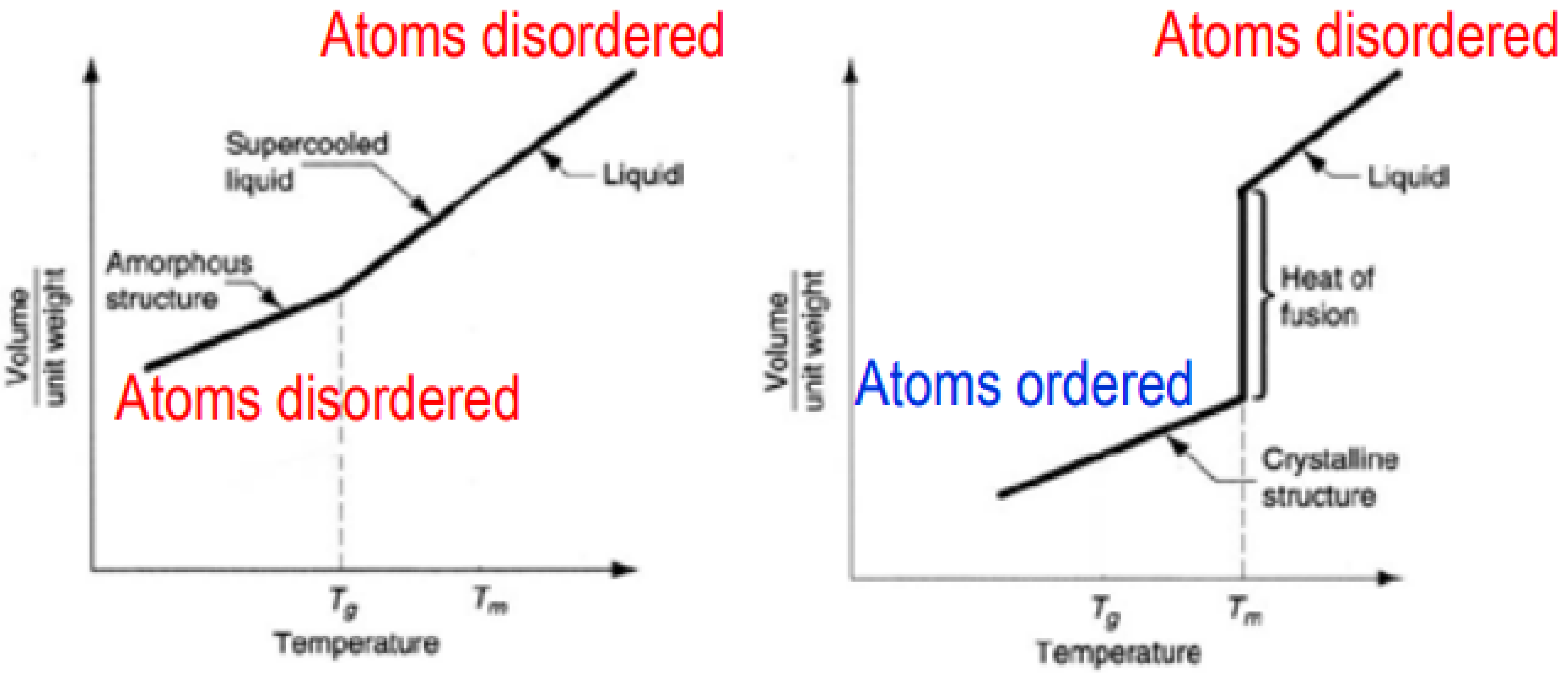


Two-dimensional schemes of the structure of (a) crystalline silicon dioxide and (b) non-crystalline silicon dioxide.

ATOMIC STRUCTURE OF MATERIALS

THERMAL BEHAVIOUR OF CRYSTALLINE AND AMORPHOUS MATERIALS

- There is a great difference between in the **phase transition characteristics** between the amorphous materials and the crystalline materials.



Characteristic change in volume for a pure metal (a crystalline structure), compared to the same volumetric changes in glass (a noncrystalline structure).

ATOMIC STRUCTURE OF MATERIALS

NON-CRYSTALLINE OR AMORPHOUS MATERIALS

Many materials are non-crystalline

- Water and air have non-crystalline structures
- A metal loses its crystalline structure when melted

- **Important engineering materials have non-crystalline forms in their solid state**

- Many plastics
- Rubber
- Glass – a typical amorphous material and often described as a supercooled liquid

ATOMIC STRUCTURE OF MATERIALS

CRYSTALLINE MATERIALS

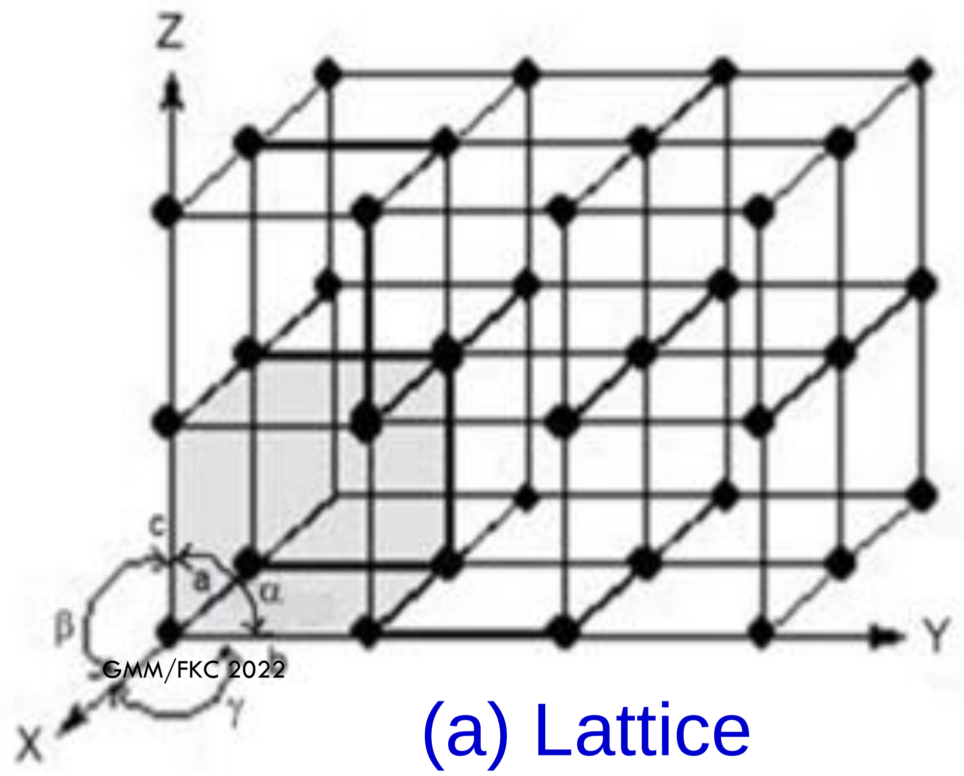
- **Crystalline** – atoms or molecules arranged in ***regular***, ***repetitive*** and ***symmetrical*** patterns ***periodic*** in 3D. This type of structure is typical of metals, many ceramics and some polymers

⇒ Certain materials may consist of single crystals (e.G. Quartz crystals for timers; and silicon crystals for semi-conductors) – they are termed ***monocrystalline***

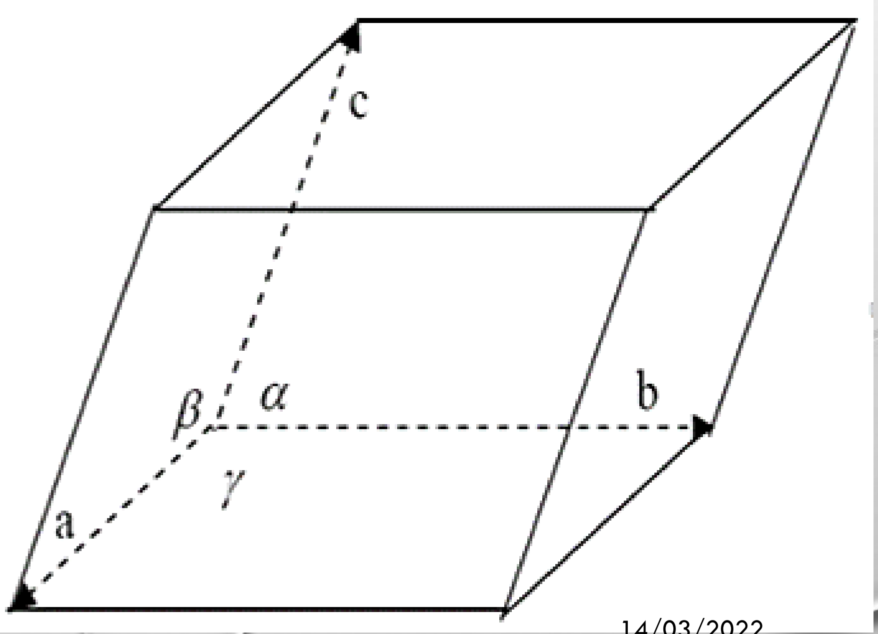
⇒ Those consisting of many crystals and are called ***polycrystalline***.

ATOMIC ARRANGEMENT IN CRYSTALS

- Groups of atoms form a repetitive pattern and the repetitive entities called **unit cell**s.
- Is the basic structural unit or building block of the crystal structure and defines the crystal structure by virtue of its geometry and the atom positions within



(a) Lattice



(b) Unit Cell

ATOMIC ARRANGEMENT IN CRYSTALS

- The space lattice points in a crystal are occupied by atoms.
- The position of any atom in the 3D lattice can be described by a vector $r_{uvw} = u\text{a} + v\text{b} + w\text{c}$, where u, v and w are integers.

- The three unit vectors, *a*, *b*, *c* can define a cell as shown by the shaded region in Fig.(a)
- This cell is known as unit cell (Fig. b) which when repeated in the three dimensions generates the crystal structure.

CRYSTAL STRUCTURE - ATOMIC ARRANGEMENT IN CRYSTALS

- Atomic arrangements described by a system of co-ordinate axes by three vectors ***a***, ***b*** and ***c*** (not co-planar)

- ***a***, ***b*** and ***c*** connect the position atoms of the smallest volume of the crystal, which characterises the arrangement and positions of atoms, called a unit cell.

- The quantities ***a***, ***b*** and ***c*** (the magnitudes of the three system vectors) and the three angles *α*, *β* and *γ* are called lattice parameters.

ATOMIC ARRANGEMENT IN CRYSTALS

Crystal Systems

- The unit vectors a, band c are called lattice parameters.
- Based on their length equality or inequality and their orientation (the angles between them, α, β and γ) a total of 7 crystal systems can be defined in three dimensions.
- These seven crystal systems are: triclinic, monoclinic, orthorhombic, hexagonal, rhombohedral, tetragonal, and cubic.

ATOMIC ARRANGEMENT IN CRYSTALS

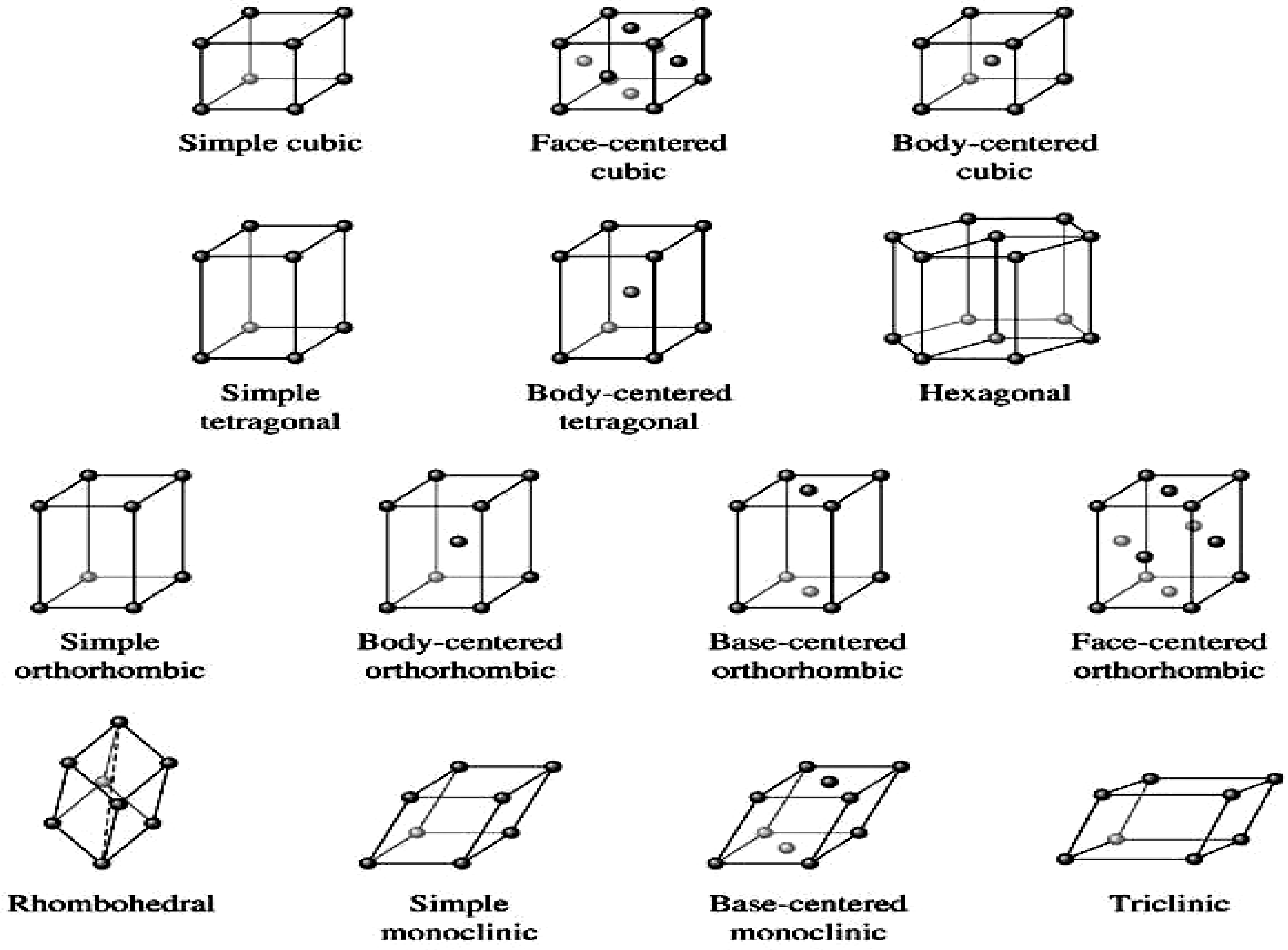
The seven systems used are summarised as follows:

1. Cubic $a = b = c$; $\alpha = \beta = \gamma = 90^o$
2. Tetragonal $a = b \neq c$; $\alpha = \beta = \gamma = 90^o$
3. Orthorhombic $a \neq b \neq c$; $\alpha = \beta = \gamma = 90^o$
4. Rhombohedral $a = b = c$; $\alpha = \beta = \gamma \neq 90^o$
5. Hexagonal $a = b \neq c$; $\alpha = \beta = 90^o$, $\gamma = 120^o$
6. Monoclinic $a \neq b \neq c$; $\alpha = \beta = 90^o \neq \gamma$
7. Triclinic $a \neq b \neq c$; $\alpha \neq \beta \neq \gamma \neq 90^o$

CRYSTAL SYSTEMS

Fourteen Bravais Lattices grouped in **Seven** Crystal Systems:

1. ***Triclinic***
2. ***Monocline***
3. ***rhombohedral = (trigonal)***
4. ***Orthorhombic***
5. ***Hexagonal***
6. ***Tetragonal***
7. ***Cubic***



ATOMIC ARRANGEMENT IN CRYSTALS

Some Materials the Crystallise in these Crystal Systems:

Crystal system	Example
Triclinic	$K_2S_2O_8$,$K_2Cr_2O_7$
Monoclinic	As_4S_4, KNO_2,$CaSO_4.2H_2O$, β-S
Rhombohedral	Hg, Sb, As, Bi, $CaCO_3$
Hexagonal	Zn, Co, Cd, Mg, Zr, NiAs
Orthorhombic	Ga, Fe_3C, α-S
Tetragonal	In, TiO_2, β-Sn
Cubic	Au, Si, Al, Cu, Ag, Fe, NaCl

END OF LECTURE 2

TO BE CONTINUED NEXT TIME.