

# ATOMIC AND CRYSTAL STRUCTURE OF MATERIALS

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# Atomic Structure of Materials

- All materials - made of atoms – protons (+ve), neutrons (no charge), and electrons (-ve).
- 118 elements are known (ref. to Periodic Table).
- Properties depend on how atoms are arranged and bonded one to another.

# Periodic Table Of The Elements

Group→	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	
↓Period																			
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

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18								
1 <b>H</b> Hydrogen 1.00794	<div style="display: flex; justify-content: space-between;"> <div style="width: 15%;"> <p><b>C</b> Solid</p> <p><b>Hg</b> Liquid</p> <p><b>H</b> Gas</p> <p><b>Rf</b> Unknown</p> </div> <div style="width: 60%; border: 1px solid black; padding: 5px;"> <p style="text-align: center;"><b>Metals</b></p> <table style="width: 100%; border-collapse: collapse;"> <tr> <td style="background-color: yellow; text-align: center;">Alkali metals</td> <td style="background-color: orange; text-align: center;">Alkaline earth metals</td> <td style="background-color: #f08080; text-align: center;">Lanthanoids</td> <td style="background-color: #f08080; text-align: center;">Actinoids</td> <td style="background-color: #f08080; text-align: center;">Transition metals</td> <td style="background-color: #00ced1; text-align: center;">Poor metals</td> <td style="background-color: #00ff00; text-align: center;">Other nonmetals</td> <td style="background-color: #66b3ff; text-align: center;">Noble gases</td> </tr> </table> </div> <div style="width: 15%;"> <p>5 <b>B</b> Boron 10.811</p> <p>6 <b>C</b> Carbon 12.0107</p> <p>7 <b>N</b> Nitrogen 14.0067</p> <p>8 <b>O</b> Oxygen 15.9994</p> <p>9 <b>F</b> Fluorine 18.9984032</p> <p>10 <b>Ne</b> Neon 20.1797</p> <p>13 <b>Al</b> Aluminium 26.9815386</p> <p>14 <b>Si</b> Silicon 28.0855</p> <p>15 <b>P</b> Phosphorus 30.973762</p> <p>16 <b>S</b> Sulfur 32.065</p> <p>17 <b>Cl</b> Chlorine 35.453</p> <p>18 <b>Ar</b> Argon 39.948</p> </div> </div>																Alkali metals	Alkaline earth metals	Lanthanoids	Actinoids	Transition metals	Poor metals	Other nonmetals	Noble gases	2 <b>He</b> Helium 4.002602
Alkali metals	Alkaline earth metals	Lanthanoids	Actinoids	Transition metals	Poor metals	Other nonmetals	Noble gases																		
3 <b>Li</b> Lithium 6.941	4 <b>Be</b> Beryllium 9.012182																	10 <b>Ne</b> Neon 20.1797							
11 <b>Na</b> Sodium 22.98976928	12 <b>Mg</b> Magnesium 24.3050																	18 <b>Ar</b> Argon 39.948							
19 <b>K</b> Potassium 39.0983	20 <b>Ca</b> Calcium 40.078	21 <b>Sc</b> Scandium 44.955912	22 <b>Ti</b> Titanium 47.887	23 <b>V</b> Vanadium 50.9415	24 <b>Cr</b> Chromium 51.9961	25 <b>Mn</b> Manganese 54.938045	26 <b>Fe</b> Iron 55.845	27 <b>Co</b> Cobalt 58.933195	28 <b>Ni</b> Nickel 58.6934	29 <b>Cu</b> Copper 63.546	30 <b>Zn</b> Zinc 65.38	31 <b>Ga</b> Gallium 69.723	32 <b>Ge</b> Germanium 72.64	33 <b>As</b> Arsenic 74.92160	34 <b>Se</b> Selenium 78.96	35 <b>Br</b> Bromine 79.904	36 <b>Kr</b> Krypton 83.798								
37 <b>Rb</b> Rubidium 85.4678	38 <b>Sr</b> Strontium 87.62	39 <b>Y</b> Yttrium 88.90585	40 <b>Zr</b> Zirconium 91.224	41 <b>Nb</b> Niobium 92.90638	42 <b>Mo</b> Molybdenum 95.96	43 <b>Tc</b> Technetium (97.9072)	44 <b>Ru</b> Ruthenium 101.07	45 <b>Rh</b> Rhodium 102.90550	46 <b>Pd</b> Palladium 106.42	47 <b>Ag</b> Silver 107.8682	48 <b>Cd</b> Cadmium 112.411	49 <b>In</b> Indium 114.818	50 <b>Sn</b> Tin 118.710	51 <b>Sb</b> Antimony 121.760	52 <b>Te</b> Tellurium 127.60	53 <b>I</b> Iodine 126.90447	54 <b>Xe</b> Xenon 131.293								
55 <b>Cs</b> Caesium 132.9054519	56 <b>Ba</b> Barium 137.327	57-71																86 <b>Rn</b> Radon (222.0176)							
87 <b>Fr</b> Francium (223)	88 <b>Ra</b> Radium (226)	89-103																118 <b>Uuo</b> Ununoctium (294)							
72 <b>Hf</b> Hafnium 178.49	73 <b>Ta</b> Tantalum 180.94788	74 <b>W</b> Tungsten 183.84	75 <b>Re</b> Rhenium 186.207	76 <b>Os</b> Osmium 190.23	77 <b>Ir</b> Iridium 192.217	78 <b>Pt</b> Platinum 195.084	79 <b>Au</b> Gold 196.966569	80 <b>Hg</b> Mercury 200.59	81 <b>Tl</b> Thallium 204.3833	82 <b>Pb</b> Lead 207.2	83 <b>Bi</b> Bismuth 208.98040	84 <b>Po</b> Polonium (208.9824)	85 <b>At</b> Astatine (209.9871)	86 <b>Rn</b> Radon (222.0176)											
104 <b>Rf</b> Rutherfordium (261)	105 <b>Db</b> Dubnium (262)	106 <b>Sg</b> Seaborgium (266)	107 <b>Bh</b> Bohrium (264)	108 <b>Hs</b> Hassium (277)	109 <b>Mt</b> Meitnerium (268)	110 <b>Ds</b> Darmstadtium (271)	111 <b>Rg</b> Roentgenium (272)	112 <b>Uub</b> Ununbium (285)	113 <b>Uut</b> Ununtrium (284)	114 <b>Uuq</b> Ununquadium (289)	115 <b>Uup</b> Ununpentium (288)	116 <b>Uuh</b> Ununhexium (292)	117 <b>Uus</b> Ununseptium	118 <b>Uuo</b> Ununoctium (294)											

For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses.

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57 <b>La</b> Lanthanum 138.90547	58 <b>Ce</b> Cerium 140.116	59 <b>Pr</b> Praseodymium 140.90785	60 <b>Nd</b> Neodymium 144.242	61 <b>Pm</b> Promethium (145)	62 <b>Sm</b> Samarium 150.36	63 <b>Eu</b> Europium 151.964	64 <b>Gd</b> Gadolinium 157.25	65 <b>Tb</b> Terbium 158.92535	66 <b>Dy</b> Dysprosium 162.500	67 <b>Ho</b> Holmium 164.93032	68 <b>Er</b> Erbium 167.259	69 <b>Tm</b> Thulium 168.93421	70 <b>Yb</b> Ytterbium 173.054	71 <b>Lu</b> Lutetium 174.9688
89 <b>Ac</b> Actinium (227)	90 <b>Th</b> Thorium 232.03806	91 <b>Pa</b> Protactinium 231.03688	92 <b>U</b> Uranium 238.02891	93 <b>Np</b> Neptunium (237)	94 <b>Pu</b> Plutonium (244)	95 <b>Am</b> Americium (243)	96 <b>Cm</b> Curium (247)	97 <b>Bk</b> Berkelium (247)	98 <b>Cf</b> Californium (251)	99 <b>Es</b> Einsteinium (252)	100 <b>Fm</b> Fermium (257)	101 <b>Md</b> Mendelevium (258)	102 <b>No</b> Nobelium (259)	103 <b>Lr</b> Lawrencium (262)

# 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.

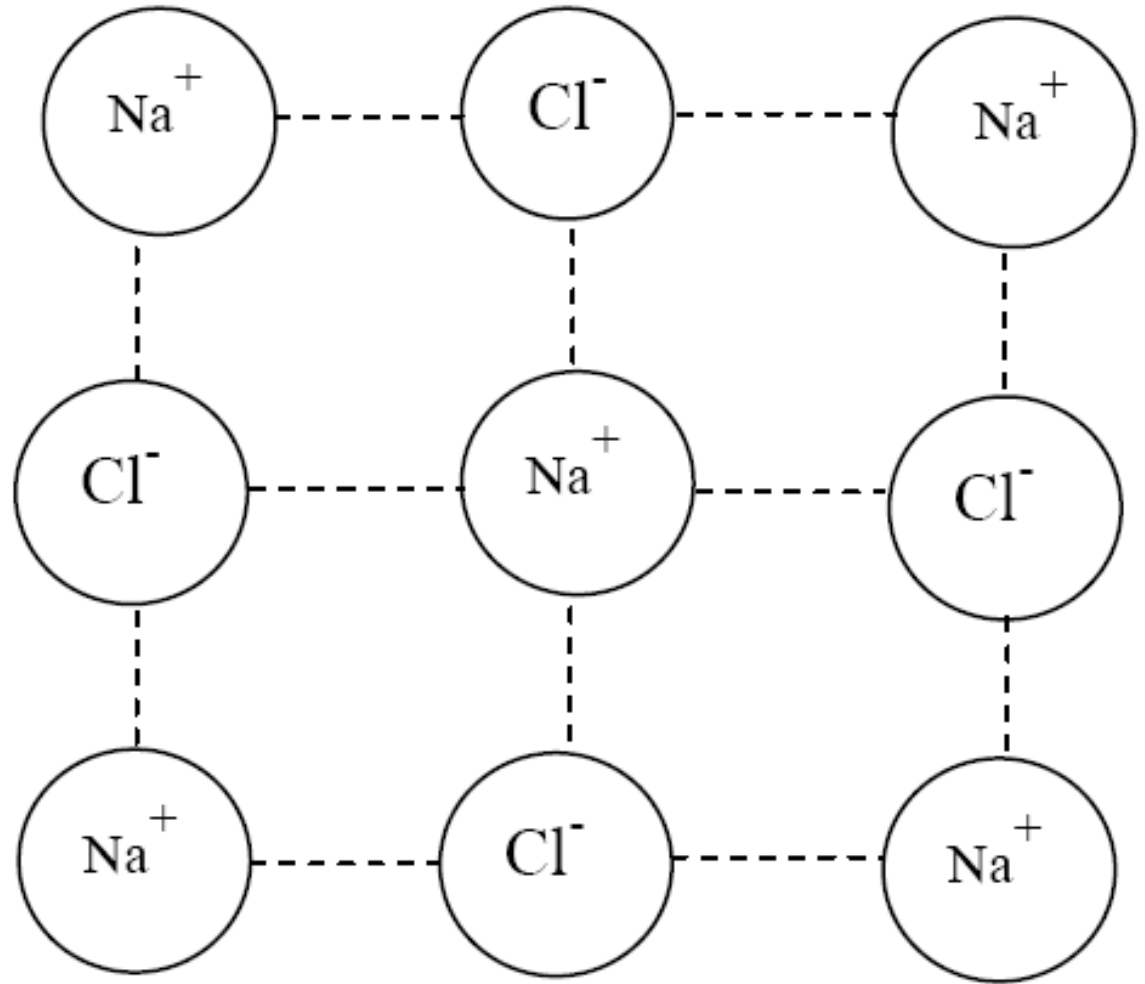
# Atomic Structure of Materials

## Ionic Bond

- Simplest type of bond
- From Electrostatic or Coulombic forces (of attraction) between +ve and -ve ions in solid crystals
- Example: Sodium Chloride (Common Salt, NaCl)
- $\text{Na}^+$  ions are surrounded by six  $\text{Cl}^-$  and
- Similarly, a  $\text{Cl}^-$  ion is surrounded by six  $\text{Na}^+$  ions.

# Atomic Structure of Materials

## 2D View of NaCl Structure



# Atomic Structure of Materials

- 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.

# 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.

# Atomic Structure of Materials

Examples:

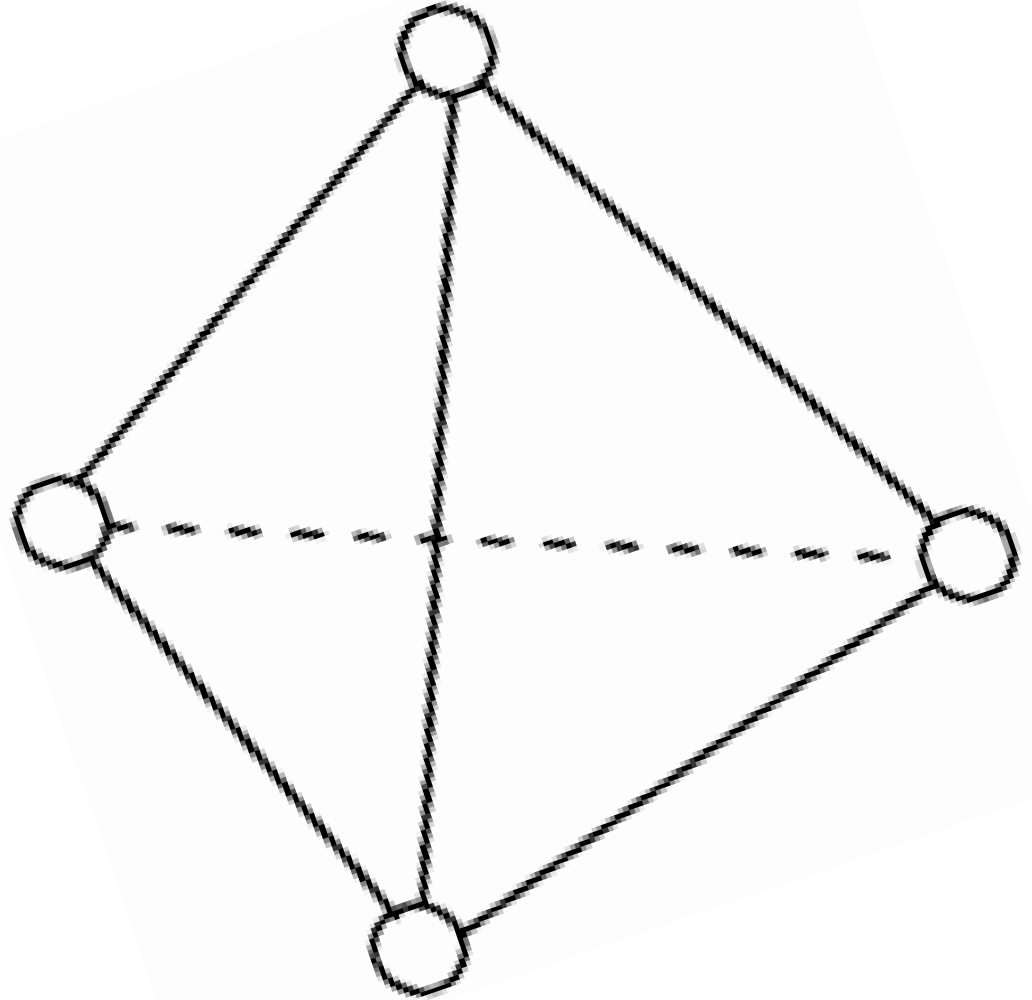
## 1. Diamond :

- 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

## 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°C).

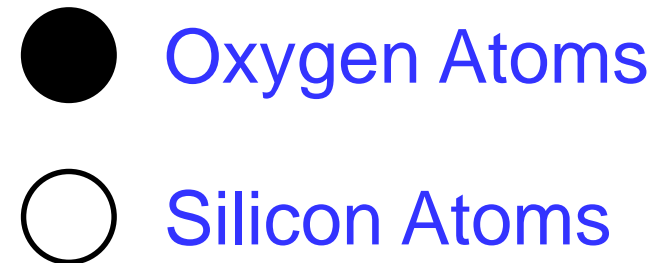
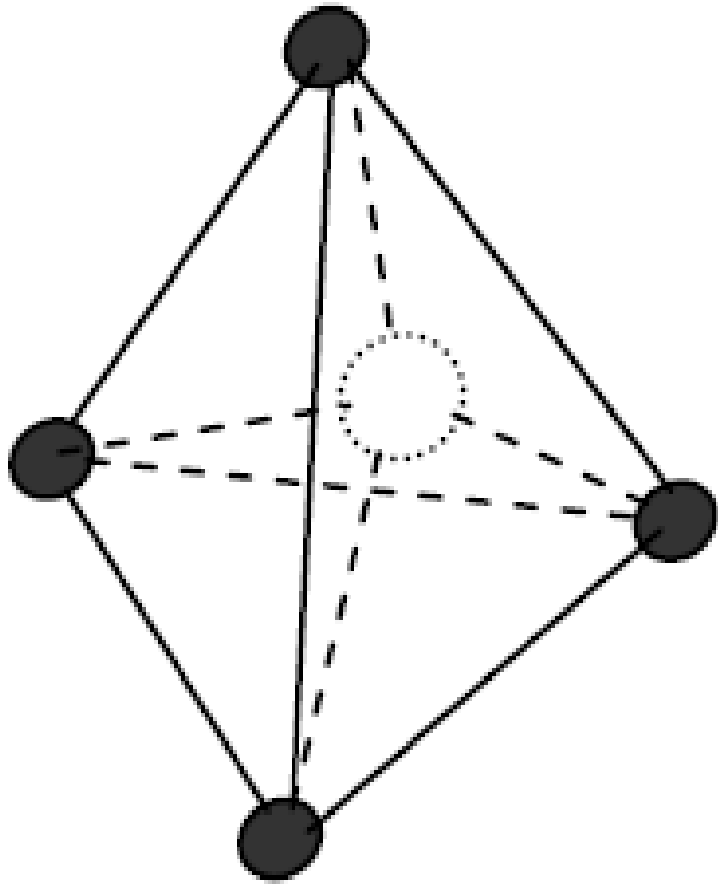


# Atomic Structure of Materials

## 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, tetrahedra are in zig-zag or random manner (although joined at the corners).

# Atomic Structure of Materials



- Because of the covalent nature of the Si-O bonds, silica is a very strong solid with a melting point of about 1710°C.

# Atomic Structure of Materials

## 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  $\text{Na}^+$  and  $\text{K}^+$  occupy the voids between the tetrahedra in glass.

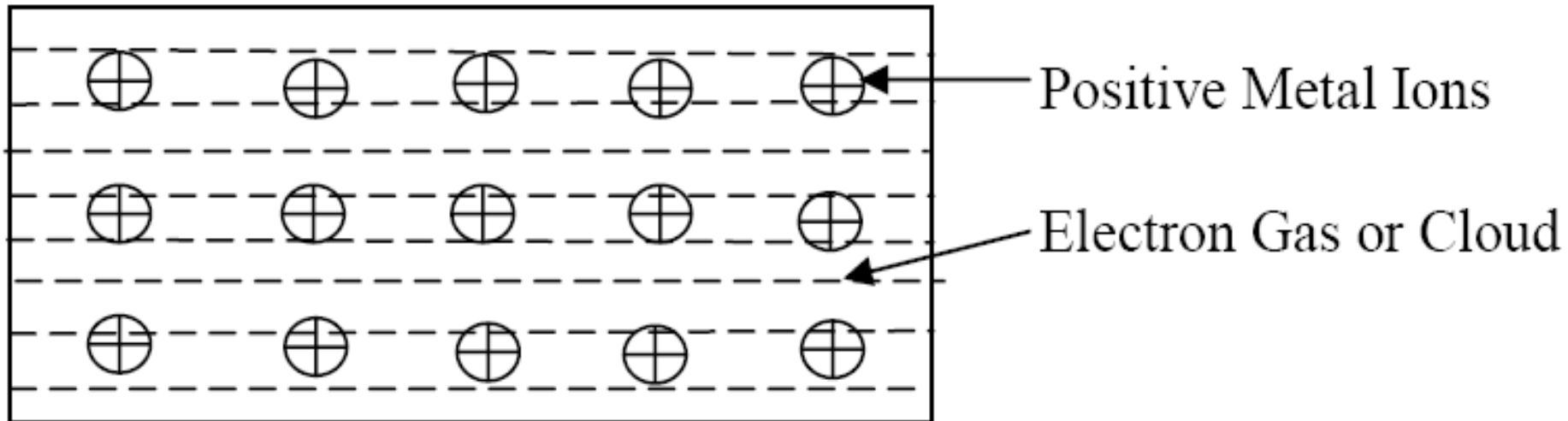
# Atomic Structure of Materials

## 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.

# Atomic Structure of Materials

## Metallic Bond



# Atomic Structure of Materials

## Result:

- 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

## Van der Waals Bond

- Weak bond
- 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

## Van der Waals 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:  $0^{\circ}\text{C} < \text{m. p.} < 400^{\circ}\text{C}$ .

# 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.

# Atomic Structure of Materials

- 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.

# Crystal Structures

**Solid materials = crystalline or amorphous**

- **Crystalline** – atoms or molecules arranged in *regular, repetitive* and *symmetrical* patterns *periodic* in 3D.
  - ⇒ 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.

# Crystal Structures

**Solid materials = crystalline or amorphous**

- **Amorphous** – though solid, they remain liquid in their internal arrangement of molecules – e.g. glass, which is described as a “super cooled liquid.”

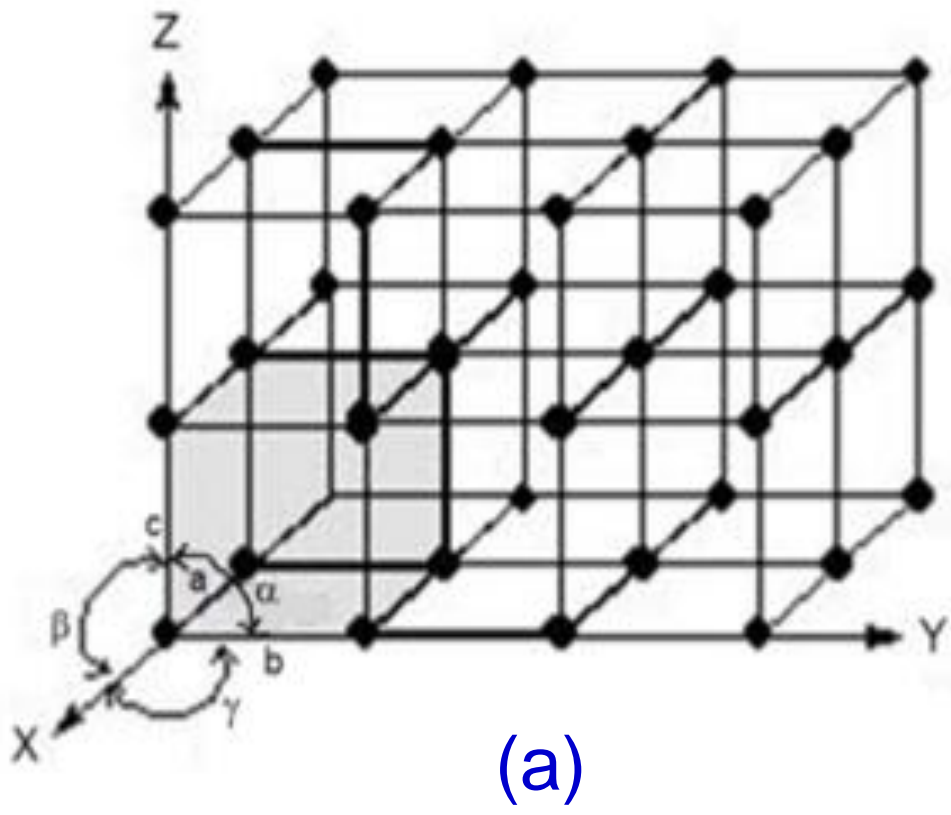
# Atomic Arrangement in crystals

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

***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.

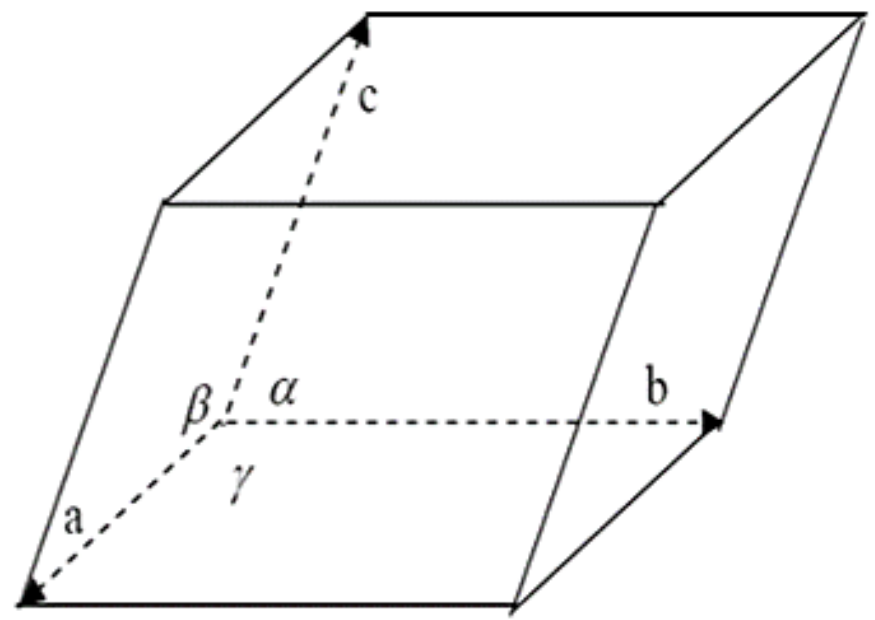
The quantities ***a***, ***b*** and ***c*** (the magnitudes of the three system vectors) and the three angles  $\alpha$ ,  $\beta$  and  $\gamma$  are called lattice parameters.

# Atomic Arrangement in crystals



(a)

Unit Cell



(b)

# 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  $r_{uvw} = ua + vb + wc$ , 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.

# Atomic Arrangement in crystals

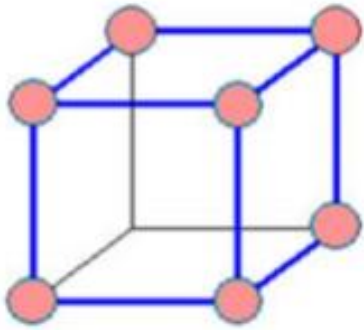
## Crystal Systems

### Bravais lattices

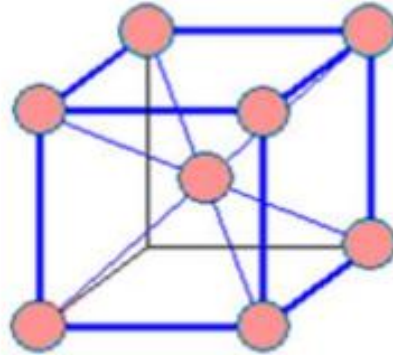
- The unit vectors  $a$ ,  $b$  and  $c$  are called lattice parameters.
- Based on their length equality or inequality and their orientation (the angles between them,  $\alpha$ ,  $\beta$  and  $\gamma$ ) a total of 7 crystal systems can be defined.
- With the centring (face, base and body centring) added to these, 14 kinds of 3D lattices, known as **Bravais lattices**, can be generated.

# Atomic Arrangement in crystals

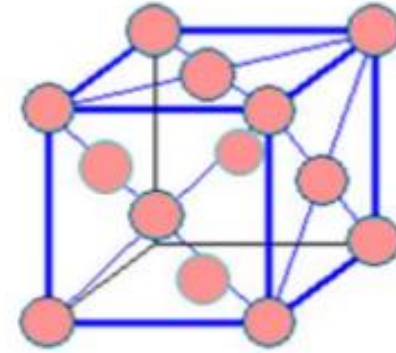
Cubic:  $a = b = c$ ,  $\alpha = \beta = \gamma = 90^\circ$



Simple cubic

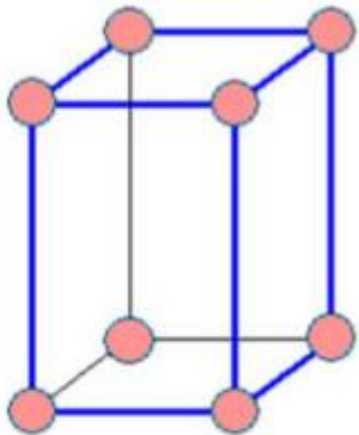


Body-centered cubic (BCC)

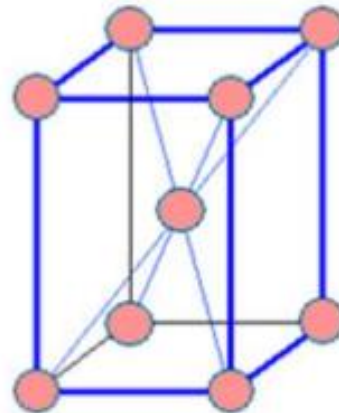


Face-centered cubic (FCC)

Tetragonal:  $a = b \neq c$ ,  $\alpha = \beta = \gamma = 90^\circ$



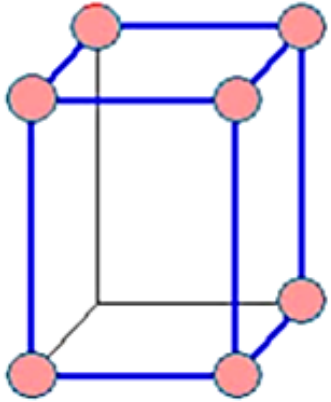
Simple Tetragonal



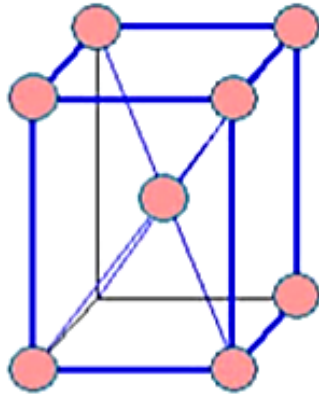
Body-centered Tetragonal (BCT)

# Atomic Arrangement in crystals

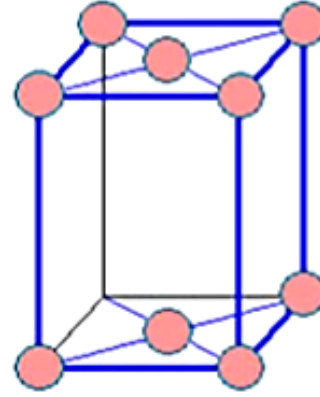
Orthorhombic:  $a \neq b \neq c, \alpha = \beta = \gamma = 90^\circ$



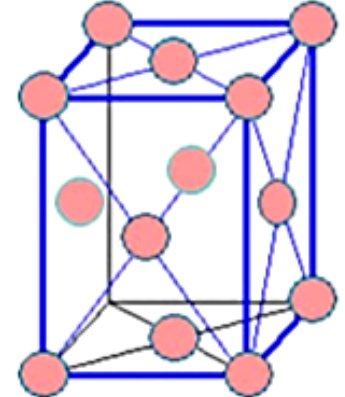
Simple



Body-centered

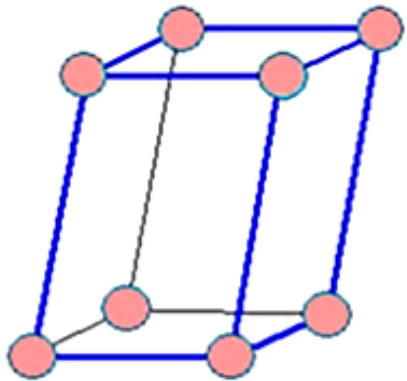


Base-centered

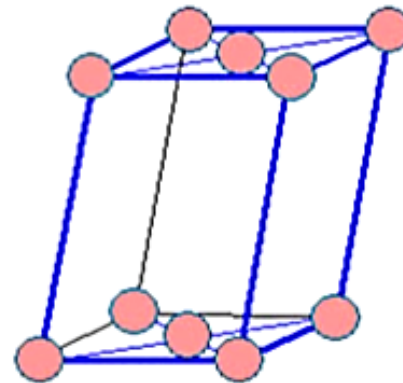


Face-centered

Monoclinic:  $a \neq b \neq c, \alpha = \gamma = 90^\circ \neq \beta$

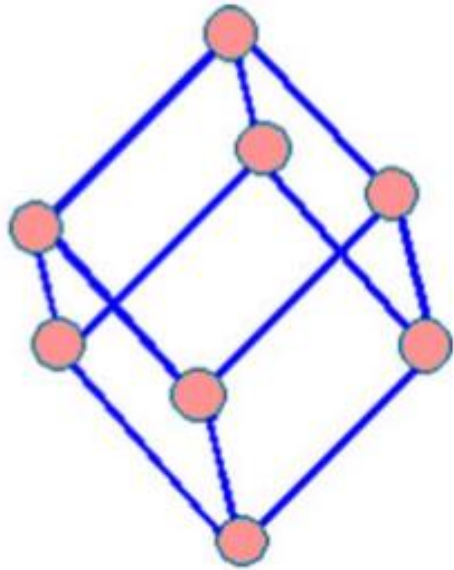


Simple  
monoclinic



Base-centered  
monoclinic

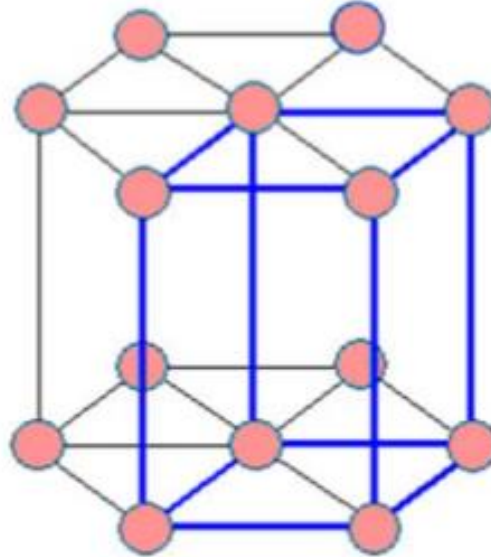
# Atomic Arrangement in crystals



Rhombohedral

$$a = b = c$$

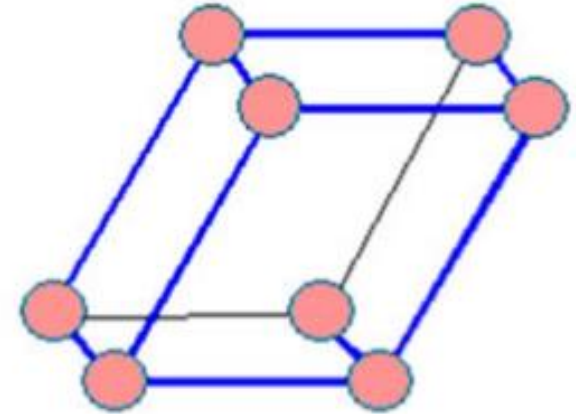
$$\alpha = \beta = \gamma \neq 90^\circ$$



Hexagonal

$$a = b \neq c$$

$$\alpha = \beta = 90^\circ \gamma = 120^\circ$$



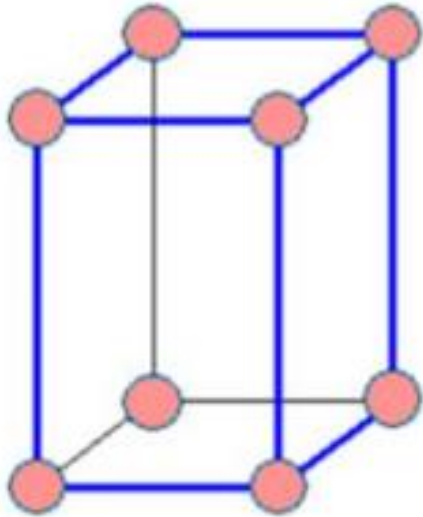
Triclinic

$$a \neq b \neq c$$

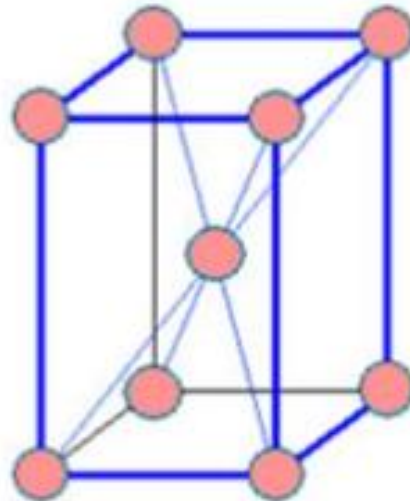
$$\alpha \neq \beta \neq \gamma \neq 90^\circ$$

# Atomic Arrangement in crystals

Tetragonal:  $a = b \neq c$ ,  $\alpha = \beta = \gamma = 90^\circ$



Simple  
Tetragonal



Body-centered  
Tetragonal (BCT)

# Atomic Arrangement in crystals

The seven systems used are summarised as follows:

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

# 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	$As_4S_4, KNO_2, CaSO_4 \cdot 2H_2O, \beta\text{-S}$
Rhombohedral	Hg, Sb, As, Bi, $CaCO_3$
Hexagonal	Zn, Co, Cd, Mg, Zr, NiAs
Orthorhombic	Ga, $Fe_3C, \alpha\text{-S}$
Tetragonal	In, $TiO_2, \beta\text{-Sn}$
Cubic	Au, Si, Al, Cu, Ag, Fe, NaCl



*To be continued  
next time*



*The End*

*To be continued next time.*