

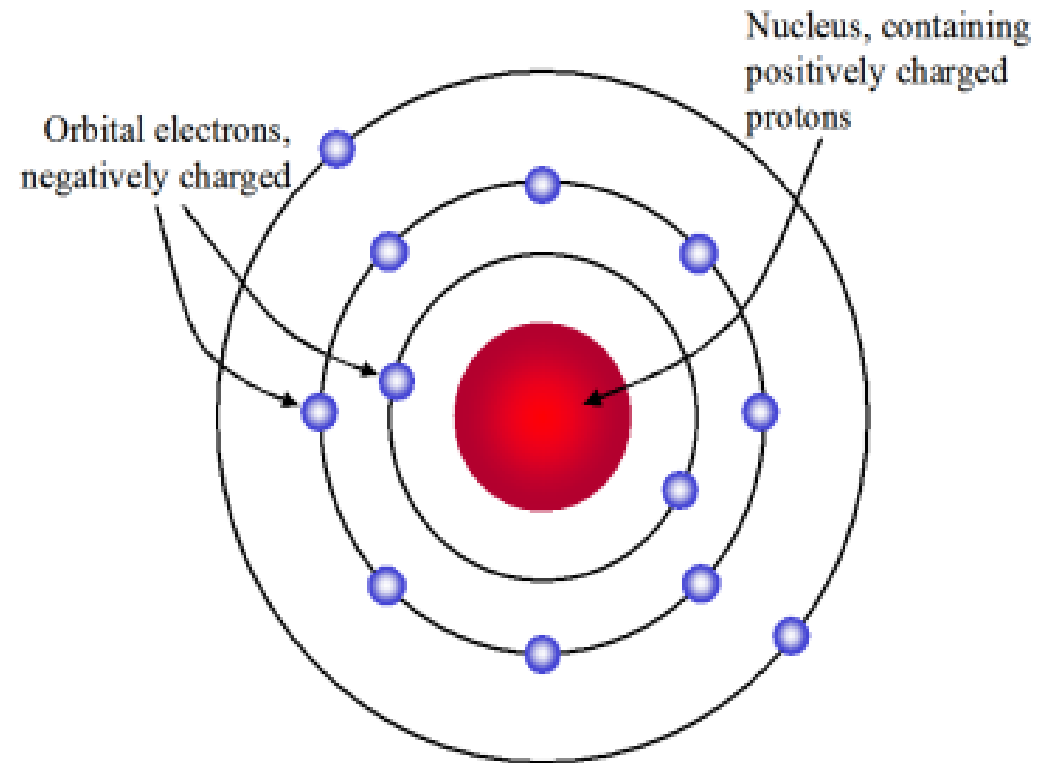
ATOMIC AND CRYSTAL STRUCTURE OF MATERIALS

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Atomic Structure of Materials

- All materials - made of atoms
- Protons and Neutrons are much larger than electrons. Protons have a positive(+) charge, neutrons have no charge and electrons have a negative(-) charge.
- Electrons exist in separate orbitals or energy states surrounding the nucleus.
- 118 elements are known (ref. to Periodic Table).
- Properties depend on how atoms are **arranged** and **bonded** one to another.



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→	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

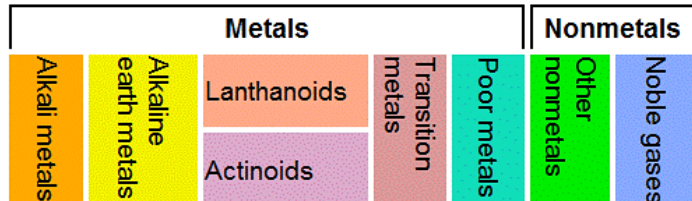
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18																	
1	H Hydrogen 1.00794																	2	He Helium 4.002602																
3	Li Lithium 6.941	4	Be Beryllium 9.012182																	5	B Boron 10.811	6	C Carbon 12.0107	7	N Nitrogen 14.0067	8	O Oxygen 15.9994	9	F Fluorine 18.9984032	10	Ne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

C Solid

Hg Liquid

H Gas

Rf Unknown



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	La Lanthanum 138.90547	58	Ce Cerium 140.116	59	Pr Praseodymium 140.90765	60	Nd Neodymium 144.242	61	Pm Promethium (145)	62	Sm Samarium 150.36	63	Eu Europium 151.964	64	Gd Gadolinium 157.25	65	Tb Terbium 158.92535	66	Dy Dysprosium 162.500	67	Ho Holmium 164.93032	68	Er Erbium 167.259	69	Tm Thulium 168.93421	70	Yb Ytterbium 173.054	71	Lu Lutetium 174.9688
89	Ac Actinium (227)	90	Th Thorium 232.03806	91	Pa Protactinium 231.03688	92	U Uranium 238.02891	93	Np Neptunium (237)	94	Pu Plutonium (244)	95	Am Americium (243)	96	Cm Curium (247)	97	Bk Berkelium (247)	98	Cf Californium (251)	99	Es Einsteinium (252)	100	Fm Fermium (257)	101	Md Mendelevium (258)	102	No Nobelium (259)	103	Lr 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
- 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 (Al_2O_3)
- Cement

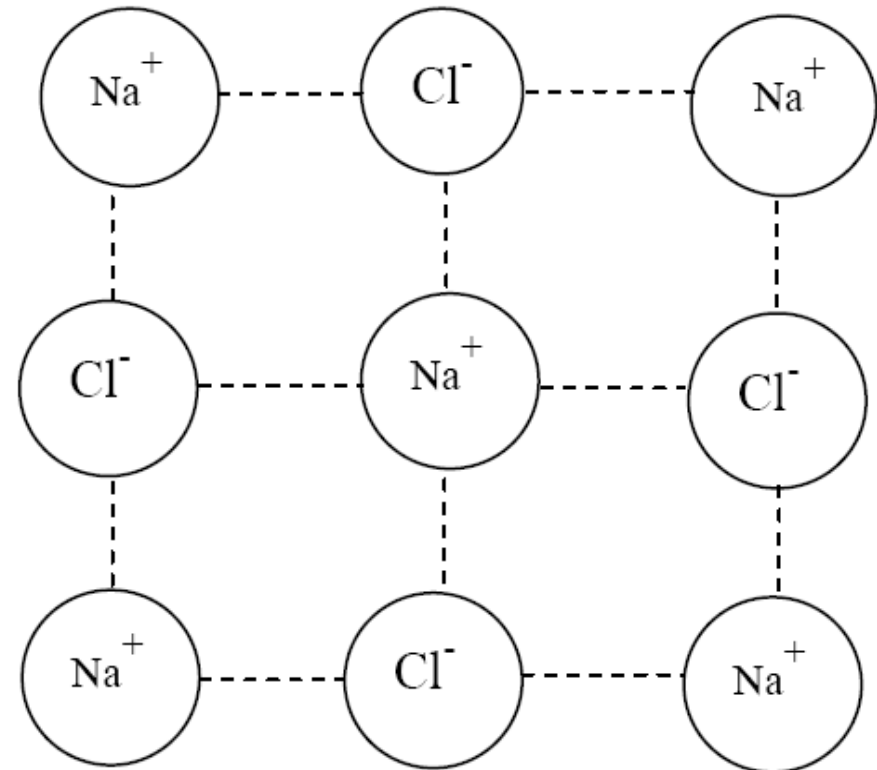
Atomic Structure of Materials

- 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

2D View of NaCl Structure

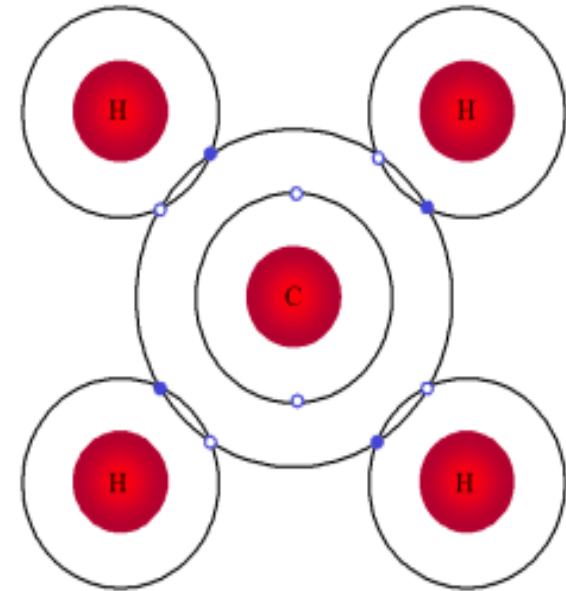
- Example: Sodium Chloride (Common Salt, NaCl)
- Na^+ ions are surrounded by six Cl^- and
- Similarly, a Cl^- ion is surrounded by six Na^+ ions.



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

Examples:

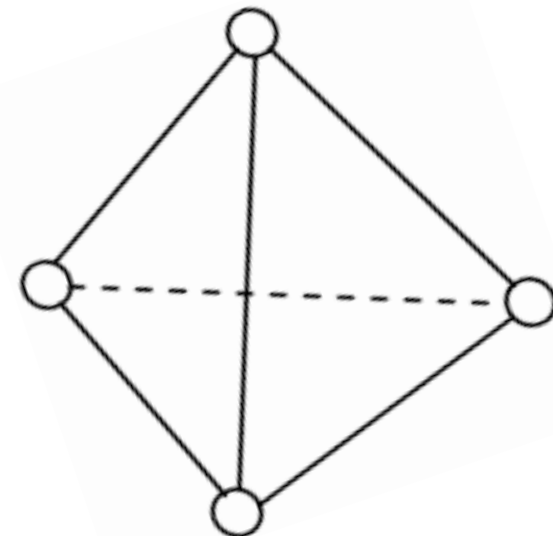
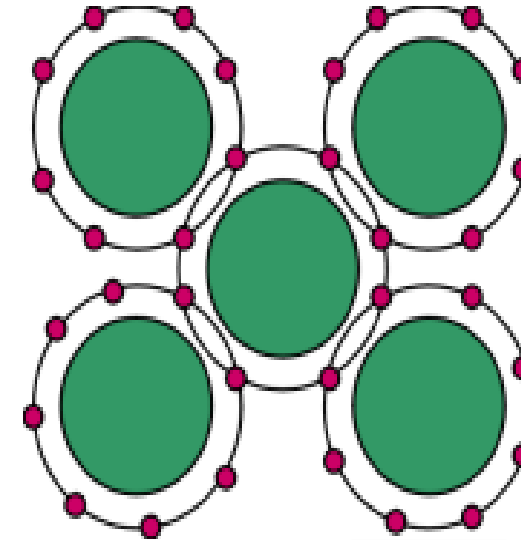
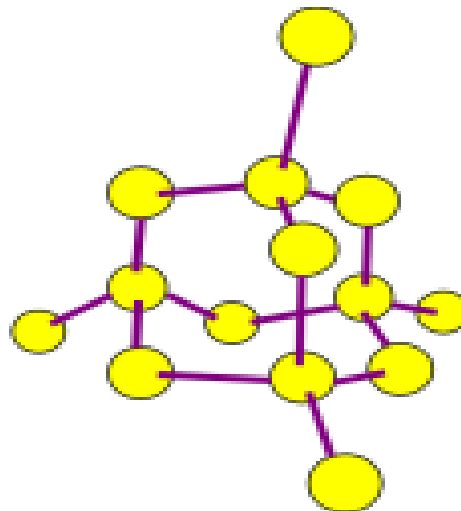
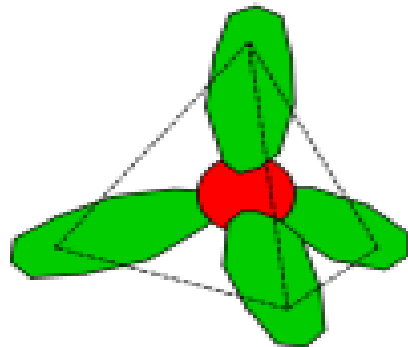
1. Diamond :

- 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).

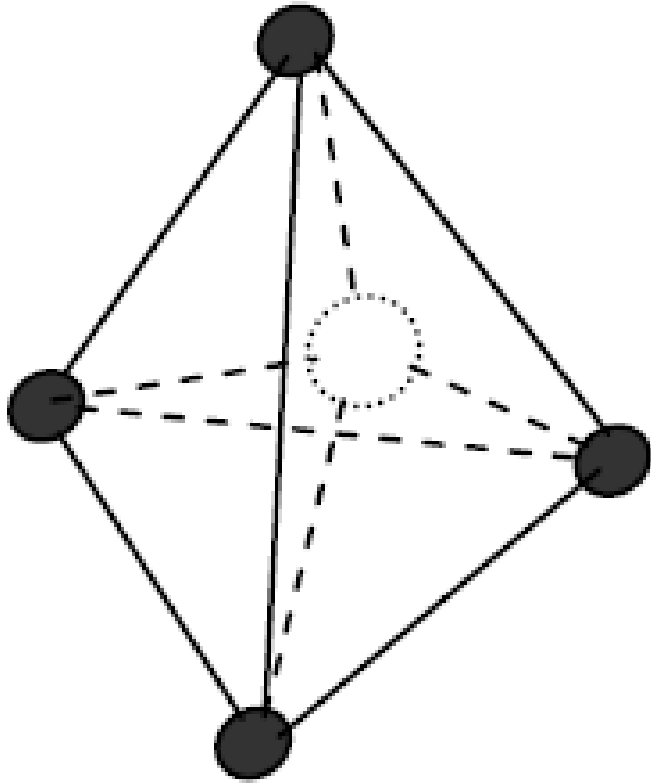


Atomic Structure of Materials

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

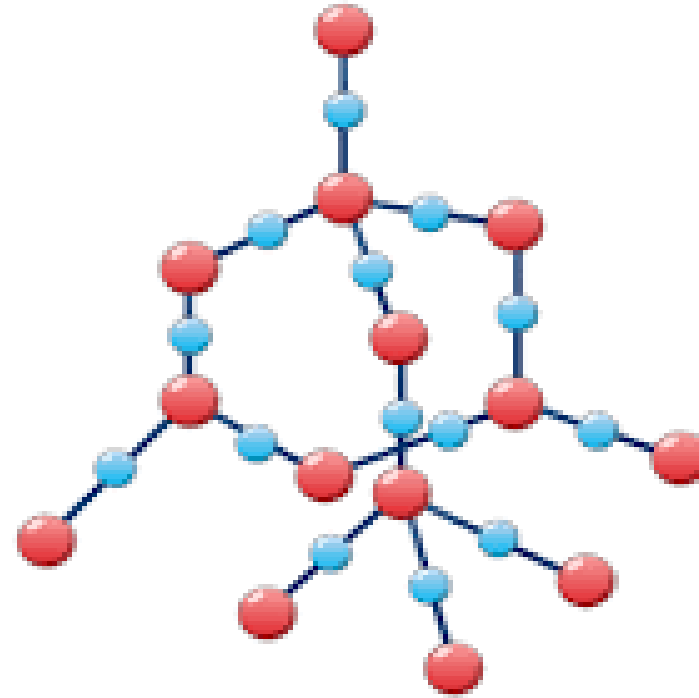
- Crystalline Silica, called quartz
- Amorphous Silica, called fused Silica or fused quartz.
- A **Si** atom is situated inside the tetrahedron with four **O** atoms at the four corners.
- In the solid, tetrahedrons or *tetrahydra* are joined at the corners.
- In amorphous silica, tetrahedra are in zig-zag or random manner (although joined at the corners).

Atomic Structure of Materials



● 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 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 Na^+ and K^+ occupy the voids between the tetrahedra in glass.

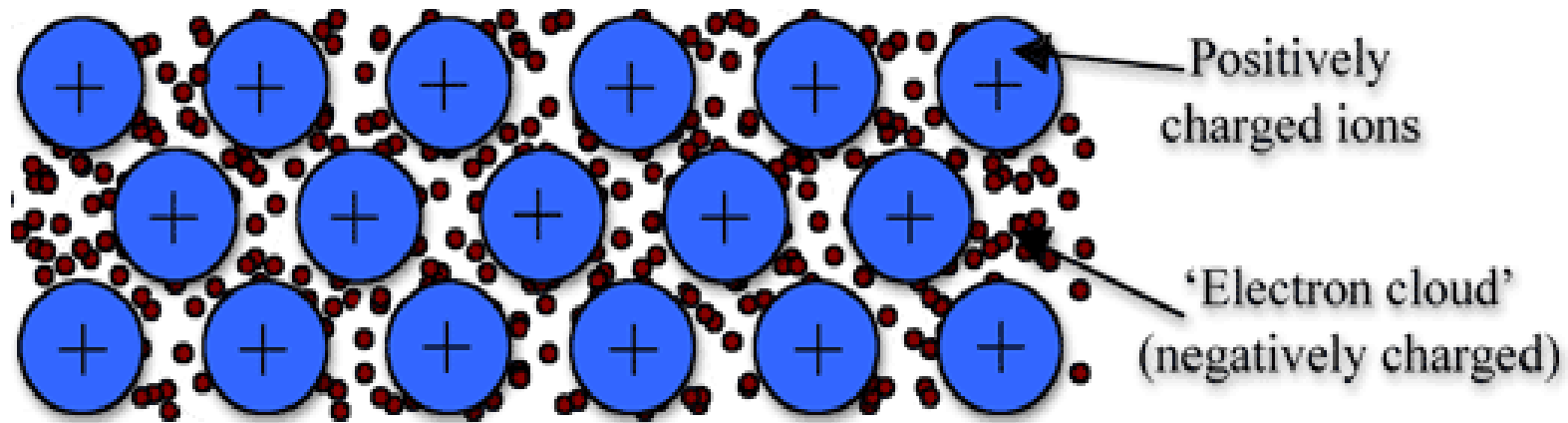
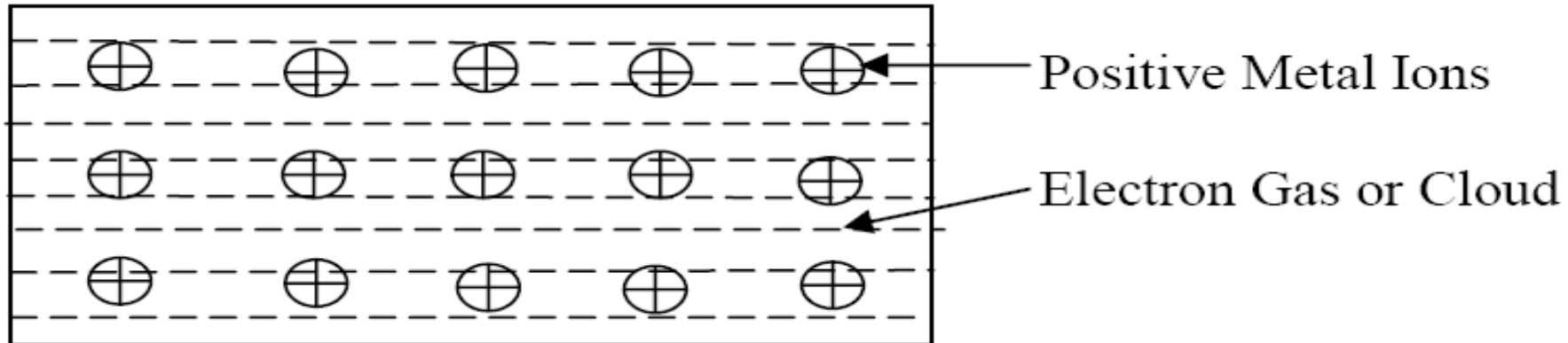
Atomic Structure of Materials

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

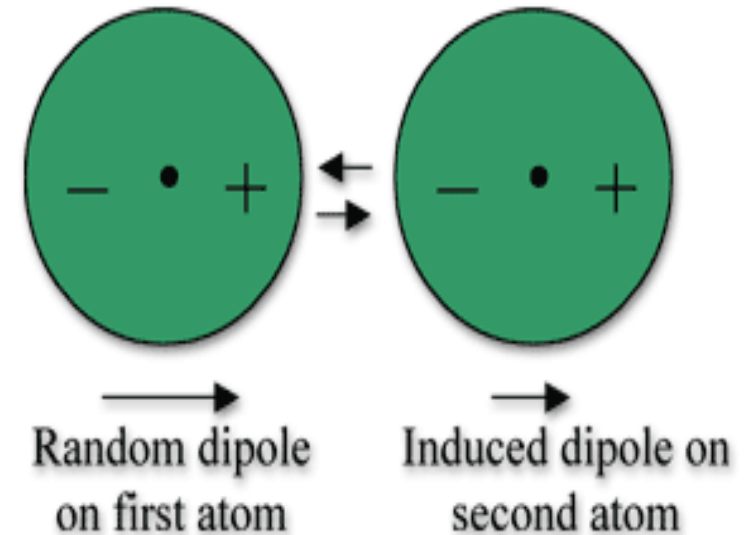
Secondary Bonding – Van Der Waals Bond

- 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

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: $0^{\circ}\text{C} < m. p. < 400^{\circ}\text{C}$.



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.
- 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

Solid materials = crystalline or amorphous

- **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.

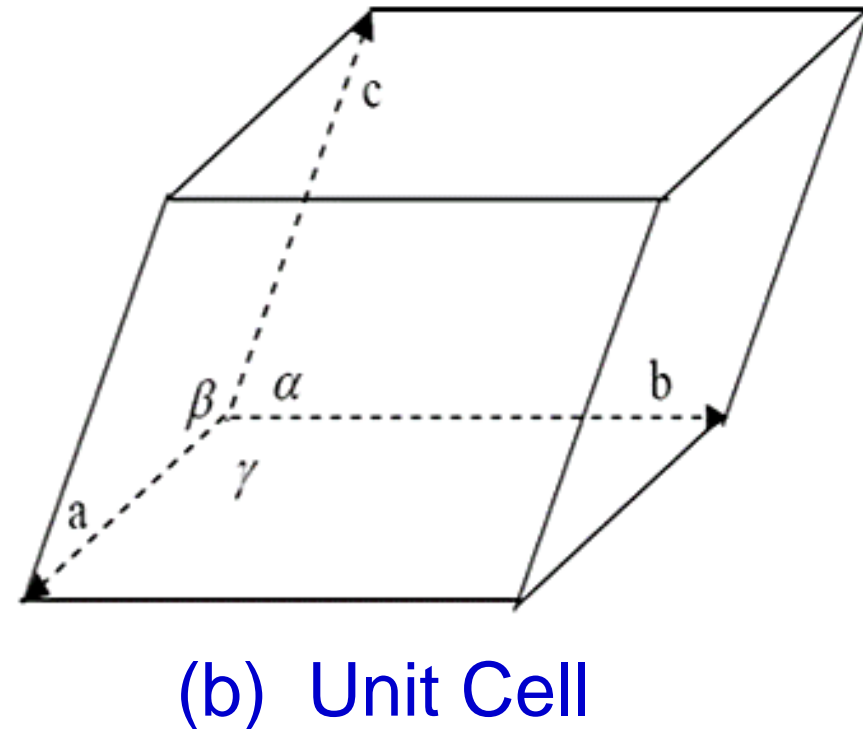
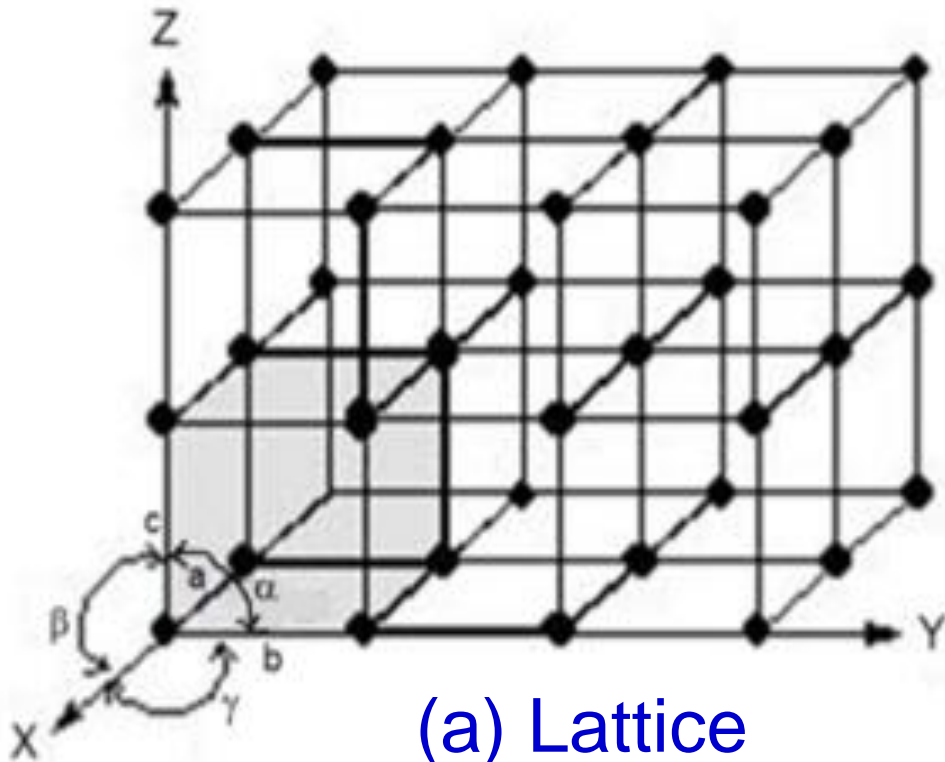
Atomic Structure of Materials

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

- Groups of atoms form a repetitive pattern and the repetitive entities called **unit cells**.
- 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



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.

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

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, 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. These collection of systems are called the **Bravais lattices**.

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 $a \neq b \neq c; \alpha \neq \beta \neq \gamma \neq 90^\circ$

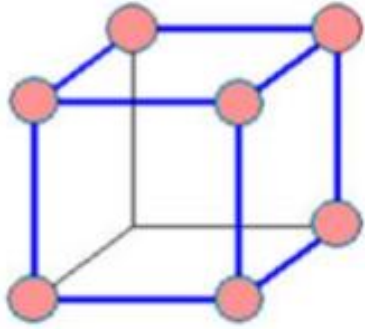
Atomic Arrangement in crystals

Bravais lattices

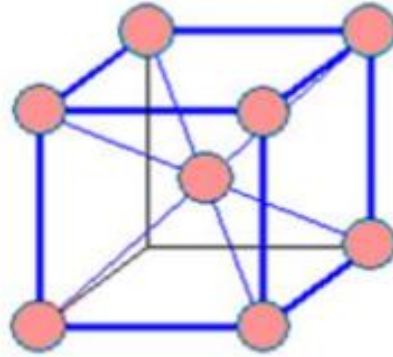
- In three-dimensional space, there are 14 Bravais lattices. These are obtained by combining one of the seven lattice systems with one of the centering types. The centering types identify the locations of the lattice points in the unit cell as follows:
- **Primitive:** lattice points on the cell corners only (sometimes called simple)
- **Base-centered:** lattice points on the cell corners with one additional point at the center of each face of one pair of parallel faces of the cell (sometimes called end-centered)
- **Body-centered:** lattice points on the cell corners, with one additional point at the center of the cell
- **Face-centered:** lattice points on the cell corners, with one additional point at the center of each of the faces of the cell

Atomic Arrangement in crystals

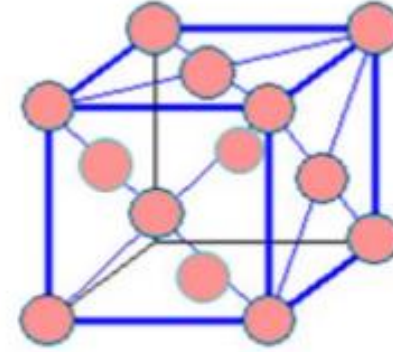
Cubic: $a = b = c$, $\alpha = \beta = \gamma = 90^\circ$



Simple
cubic

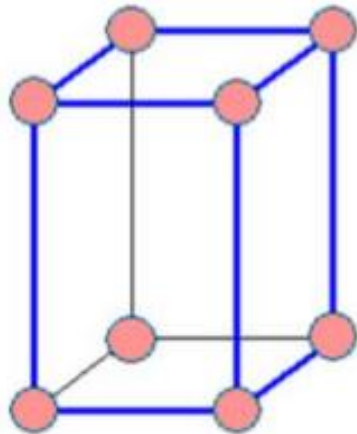


Body-centered
cubic (BCC)

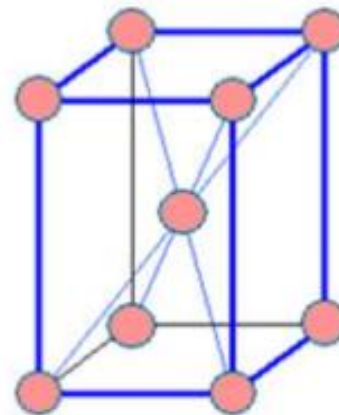


Face-centered
cubic (FCC)

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



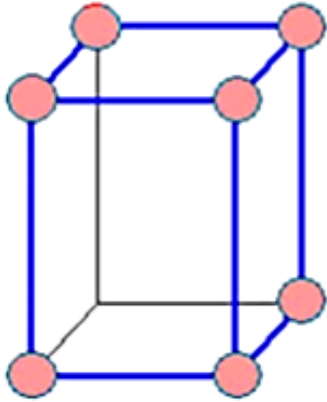
Simple
Tetragonal



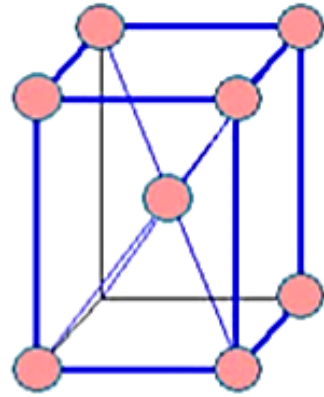
Body-centered
Tetragonal (BCT)

Atomic Arrangement in crystals

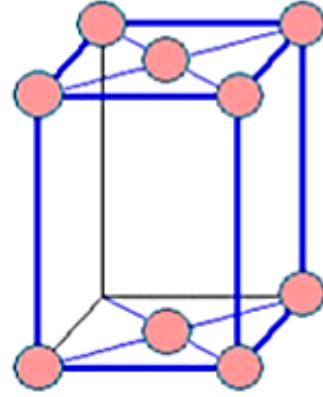
Orthorhombic: $a \neq b \neq c$, $\alpha = \beta = \gamma = 90^\circ$



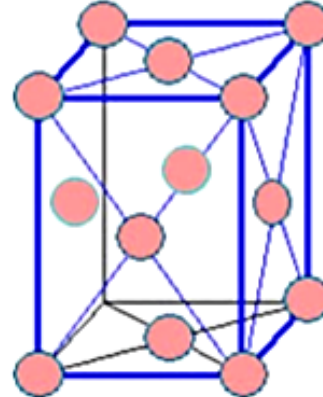
Simple



Body-centered

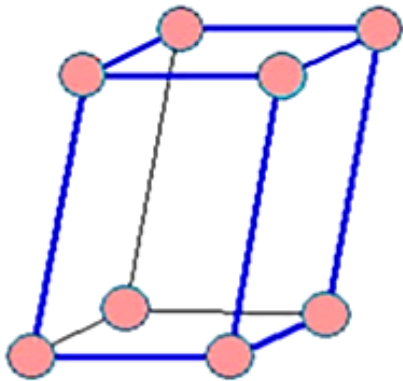


Base-centered

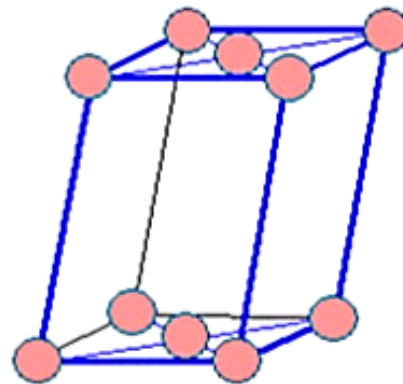


Face-centered

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

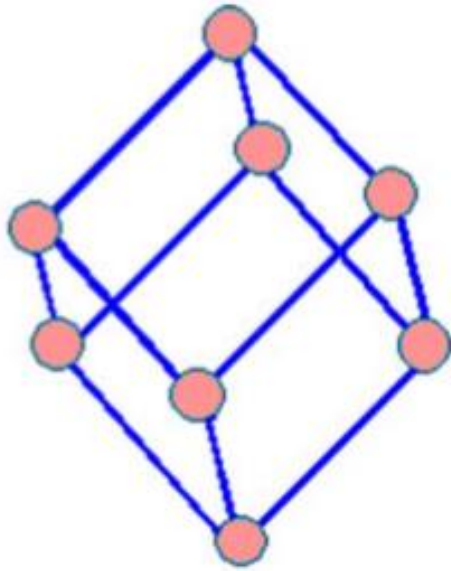


Simple
monoclinic

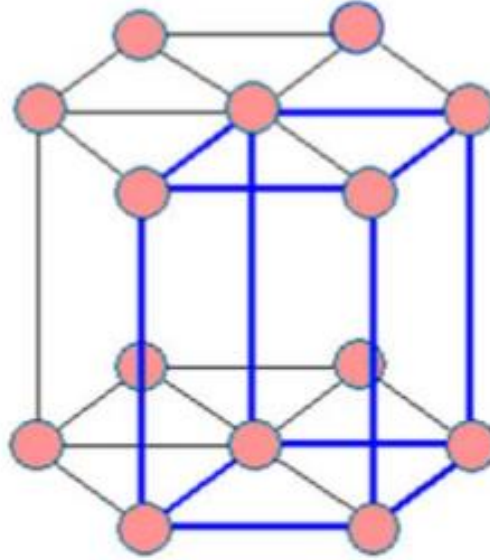


Base-centered
monoclinic

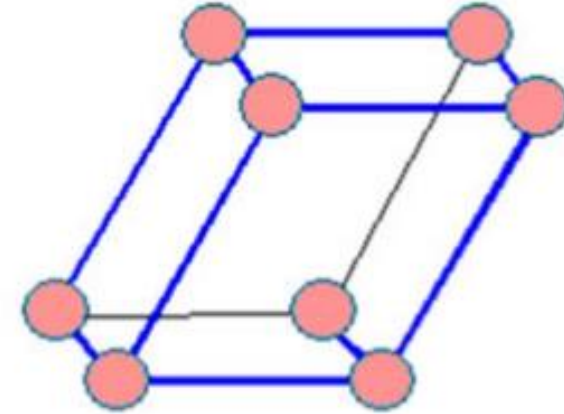
Atomic Arrangement in crystals



Rhombohedral
 $a = b = c$
 $\alpha = \beta = \gamma \neq 90^\circ$



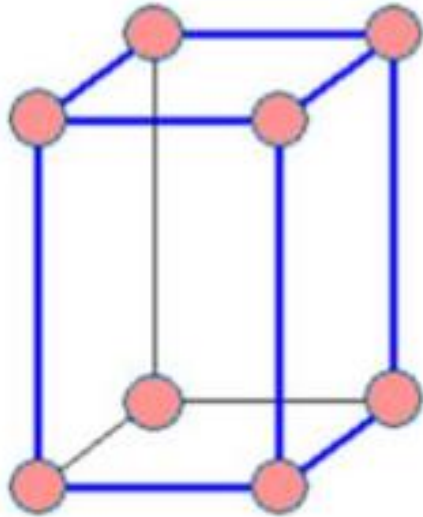
Hexagonal
 $a = b \neq c$
 $\alpha = \beta = 90^\circ \gamma = 120^\circ$



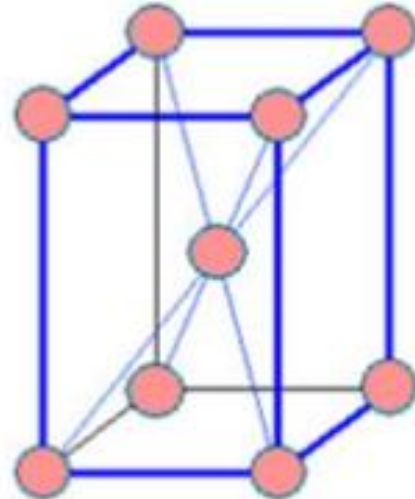
Triclinic
 $a \neq b \neq c$
 $\alpha \neq \beta \neq \gamma \neq 90^\circ$

Atomic Arrangement in crystals

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



Simple
Tetragonal



Body-centered
Tetragonal (BCT)

Atomic Arrangement in crystals

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.