# *Atomic Structure*
# *Introduction:*

An atom consists of a nucleus composed of protons and neutrons and electrons which encircle the nucleus.

The Nucleus, in the center of the atom, consists of protons and neutrons. Orbiting around the nucleus are the electrons.

♦ Protons and electrons have same and opposite charge of $1.6 \times 10^{-19}$ C.

♦ Atomic number (Z) = Number protons = number of electrons.

♦ Atomic mass (A) = proton mass + neutron mass.

♦ Isotopes are the same element having different atomic masses. Number of protons in isotopes remains same while number of neutrons varies.

♦ Atomic mass unit (amu) = 1/12 mass of Carbon 12 (12C)

♦ 1 mol of substance contains $6.023 \times 10^{23}$ (Avogadro's number) atoms or molecules.

♦ Atomic weight = 1 amu/atom (or molecule) = 1 g/mol = Wt. of $6.023 \times 10^{23}$ atoms or molecules

For example, atomic weight of copper is 63.54 amu/atom or 63.54 g/mole

• Materials ➜ Molecules ➜ Atoms

• Atoms = protons (p) + neutrons (n) + electrons (e)

• Protons and neutrons are made of quarks

## *Nonlocalized behavior of electrons in metals*

• High electrical conductivity

  - electrons move easily when E-field applied

• High thermal conductivity

  - the electrons can carry energy through metal

• High density

 - outer shell removed from atoms, so can be packed together

• High ductility

  - if metal distorted, bent, electrons can quickly move to compensate

  - metal bond is not directional

## *Quantum numbers*

Four parameters or numbers called Quantum numbers are needed to describe the distribution and position of electrons in an atom.

The first three of them (n, l, ml) describe the size, shape, and spatial orientation of the probability density distribution of electrons .

## *Principal quantum number, n*

It describes electron shells as shown in the Bohr model.

Values of n can be 1, 2, 3, 4 … corresponding to electron shells K, L, M, N …..

The value of *n* also determines the size or distance of the shells from the nucleus.

## *Azimuthal or Angular quantum number, l*

It signifies subshell or electron orbital – s, p, d, f and so on.

**, $l$** can take values of from 0 to n-1. K shell, n = 1, one s orbital. L , n =2, two orbitals, s, p. M, n =3, three orbitals s, p, d. N, n =4, four orbitals s, p, d, f and so on.

The value of l decides the shape of the orbital as shown in the figure below. s orbital (**$l$** = 0) – spherical, p (**$l$** = 1) – polar or dumbbell shaped, d (**$l$** =2 ) – double-dumbbell shaped



$l = 0$
s

$l = 1$
p

$l = 2$
d
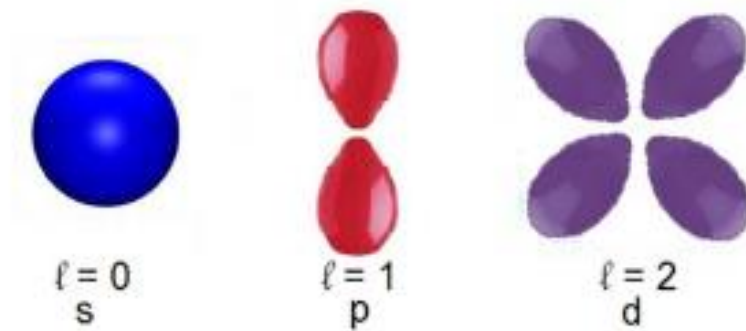
## *Electron Configuration*

The quantum mechanics principles as discussed before allow determination of electron configuration i.e. the manner in which electron states are occupied in a given atom.



$$\sum_{l=0}^{n-1} 2(2l+1)$$ Max no. of Electrons

| n =1 | 1s | | | | | | | 2 |
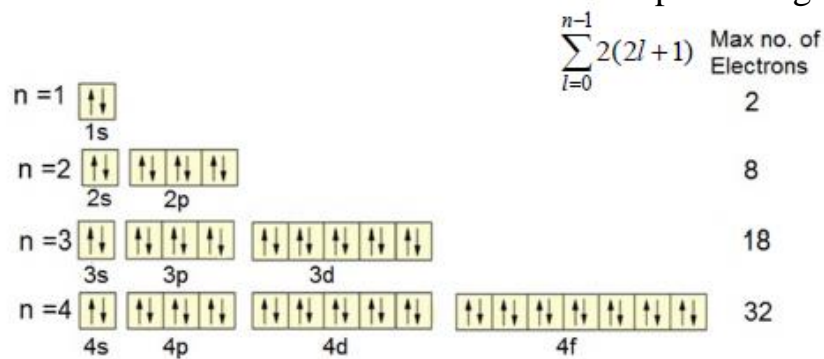
Electron configuration based on quantum numbers. Total number of electrons in a shell is $2n^2$ or
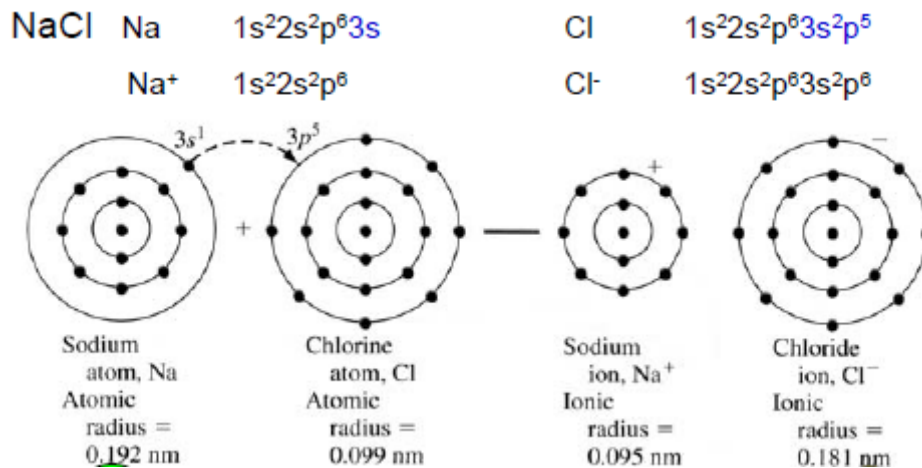
$$\sum_{l=0}^{n-1} 2(2l+1)$$

e.g. The atomic structure of sodium, atomic number 11, showing the electrons in the K, L, and M quantum shells



Na

● 11 Protons   ● 12 Neutrons   ● 11 Electrons
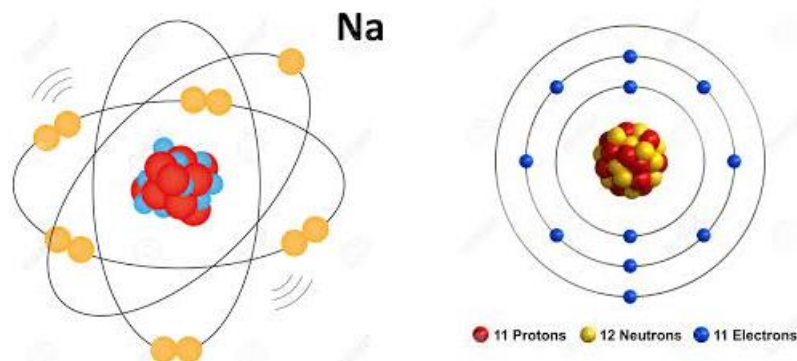
# *Types of atomic and molecular bonds*

## • *Primary atomic bonds*

1. Ionic (large interatomic forces, nondirectional, electron transfer, coulombic forces)
Typically between highly electropositive (metallic) and electronegative (nonmetallic) elements

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

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



| Sodium atom, Na | Chlorine atom, Cl | Sodium ion, $Na^+$ | Chloride ion, $Cl^-$ |
|---|---|---|---|
| Atomic radius = 0.192 nm | Atomic radius = 0.099 nm | Ionic radius = 0.095 nm | Ionic radius = 0.181 nm |

2. Covalent (large interatomic forces, localized (directional), electron sharing)
•Takes place between elements with small difference in electronegativity
- F, O, N, Cl, H, C, Si…
• *s* and *p* electrons are commonly shared to attain noble gas electron configuration
• Multiple bonds can be formed by one atom

*Hydrogen molecule*   2 H: 1s → H₂ 1s₂

H· + H· →H : H (electron –pair covalent bond)



Hydrogen molecule

Bonding interaction
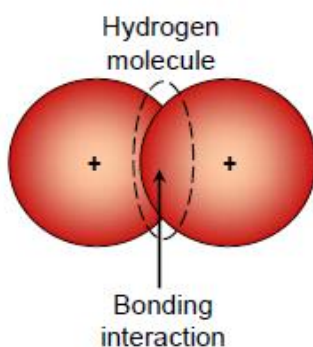
## *Carbon-containing molecules*

• C and H: hydrocarbons
• Structural formulas: $CH_4$ (methane), $C_2H_6$ (ethane), and $C_4H_{10}$ (normal butane)
• Saturated $C_nH_{2n+2}$
- strong bonds inside molecule, weak between molecules
• Unsaturated $C_nH_{2n}$, $C_nH_{2n-2}$
- generally more reactive

*Benzene (C₆H₆)*

important for some polymeric materials
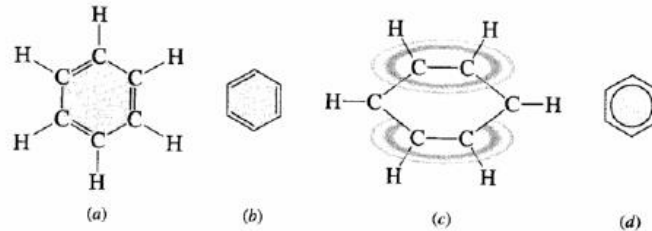


### 3. Metallic (large interatomic forces) nondirectional

metallic bond forms when atoms give up their valence electrons, 1, 2 or 3 from each atom, which then form an electron sea. The positively charged atom cores are bonded by mutual attraction to the negatively charged electrons. As the bond is not polar, metals are ductile.
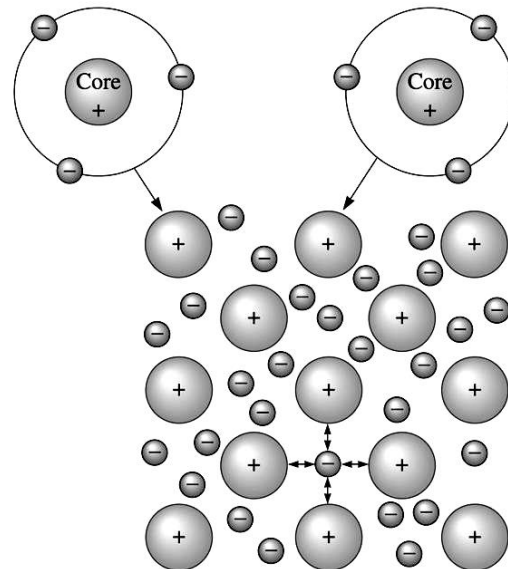


### • *Secondary atomic and molecular bonds*

Fluctuating or permanent dipoles (also called **physical bonds,or van der Waals bonds or forces)**

   - weak relatively to the primary bonding (2-5eV/atom or ion)
~ 0.1eV/atom or ~ 10 kJ/mol
   - always present, but overwhelmed by other interaction most easily observed in inert gases
   - dipoles to be considered
1. Permanent dipole bonds
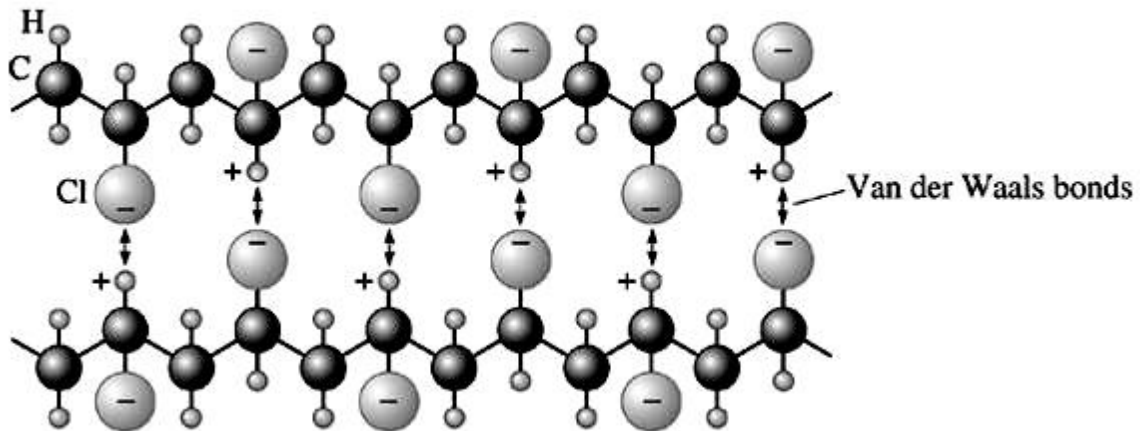2. Fluctuating dipole bonds
(Common, but weaker than primary bonding)
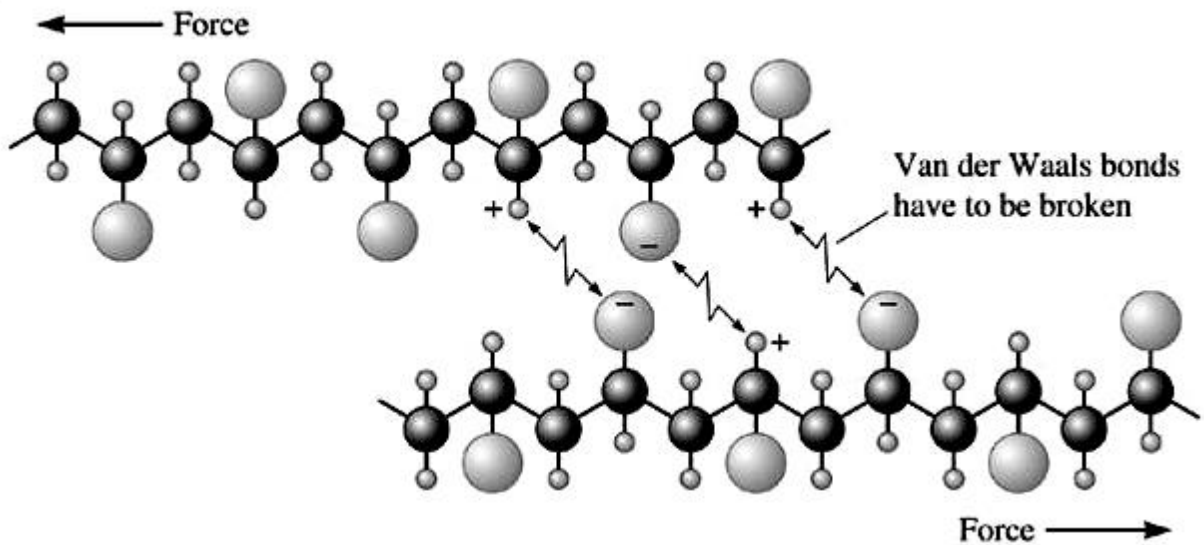    Dipole-dipole
    H-bonds

Polar molecule-induced dipole
Fluctuating dipole (weakest)

**(a)**



(a)In polyvinyl chloride (PVC), the chlorine atoms attached to the polymer chain have a negative charge and the hydrogen atoms are positively charged.
The chains are weakly bonded by van der Waals bonds. This additional bonding makes PVC stiffer,

**(b)**



(b) When a force is applied to the polymer, the week van der Waals bonds are broken and the chains slide easily past one another

### *Binding energy*
If a body has a mass *m*, then it contains an amount of energy:
$$E = mc^2$$

probably the most famous equation in physics. This means that *if* the mass of a nucleus is *less* than the mass of its constituents, then those constituents are in a *lower energy state* when they are bound together inside the nucleus.

-This difference in mass, expressed as energy (normally MeV), is the *binding energy* of those constituents inside the nucleus.

-It is found that the mass of a nucleus is always *less than* the sum of the masses of its constituent neutrons and protons (nucleons).

-What is the reason for this? Well Einstein showed that mass and energy are equivalent. The lower mass shows that the nucleons in the nucleus are in a *lower energy state* than if they were all separate, isolated particles.

-This decrease in mass (known as the mass decrement) gives the *binding energy* of the particular nucleus in terms of the equivalent *mass*.

Working in terms of the actual binding energy, we calculate as follows.

Say for example if we have a nucleus with *Z* protons and *N* neutrons and mass *MA*, where *A = Z + N* then its binding energy in MeV is given by:

*Eb(MeV) = (Zmp + Nmn - MA)* x 931.494 MeV/u

All in atomic mass units, u or *all* in nuclide masses, u

It means that there must be some force between the nucleons that binds them together in the nucleus. This is the *strong force*.

***Notes:***

o Interatomic spacing is equilibrium spacing between the centers of two atoms (at a particular temperature), equilibrium is lowest energy state, attractive and repulsive forces are balanced

o Binding (bond) energy is energy required to separate two atoms from their equilibrium spacing to an infinite distance apart, $E = mc^2$, so each time two atoms bound to each other, some mass is converted into energy, …

o Modulus of elasticity, Young's modulus, is slope of the stress strain curve in elastic region (macroscopic), can be derived from slope of force versus distance curve at interatomic spacing (microscopic)

o Coefficient of thermal expansion and melting temperature can also be explained from binding energy curve
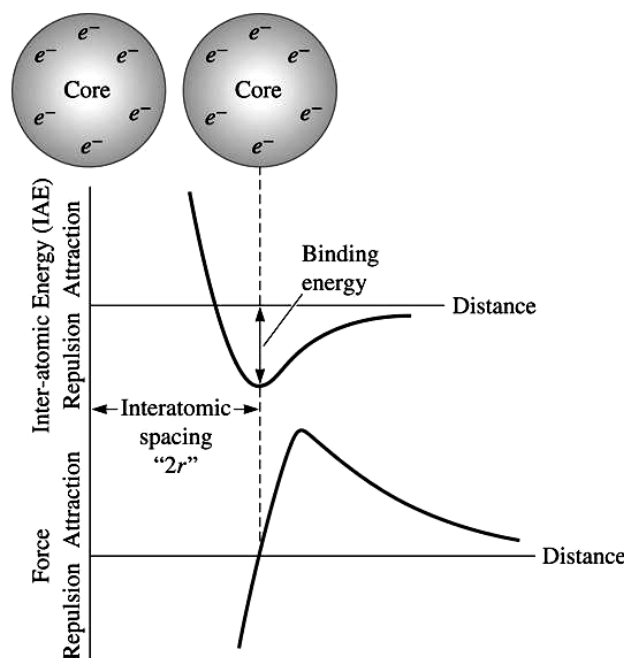
Atoms or ions are separated by equilibrium spacing that corresponds to the minimum interatomic energy for a pair of atoms or ions (or when zero force is acting to repel or attract the atoms or ions, force balance) If there is external influences, e.g. load, temperature change, equilibrium spacing will change.

## *The periodic table*

The periodic table contains valuable information about specific elements and can also help identify trends in atomic size, melting point, chemical reactivity, and other properties.

The familiar periodic table (Figure below) is constructed in accordance with the electronic structure of the elements. Not all elements in the periodic table are naturally occurring. Rows in the periodic table correspond to quantum shells, or principal quantum numbers. Columns typically refer to the number of electrons in the outermost *s* and *p* energy levels and correspond to the most common valence. In engineering, we are mostly concerned with

(a) Polymers (plastics) (primarily based on carbon, which appears in Group 4B);

(b) Ceramics (typically based on combinations of many elements appearing in

Groups 1 through 5B, and such elements as oxygen, carbon, and nitrogen); and

(c) Metallic materials (typically based on elements in Groups 1, 2 and transition

metal elements).

The **interatomic spacing** in a solid metal is *approximately* equal to the atomic diameter, or twice the atomic radius *r*. We cannot use this approach for ionically bonded materials, however, since the spacing is the sum of the two different ionic radii.

Compounds formed from two or more metals (**intermetallic compounds**) may be bonded by a mixture of metallic and ionic bonds, particularly when there is a large difference in electronegativity between the elements.
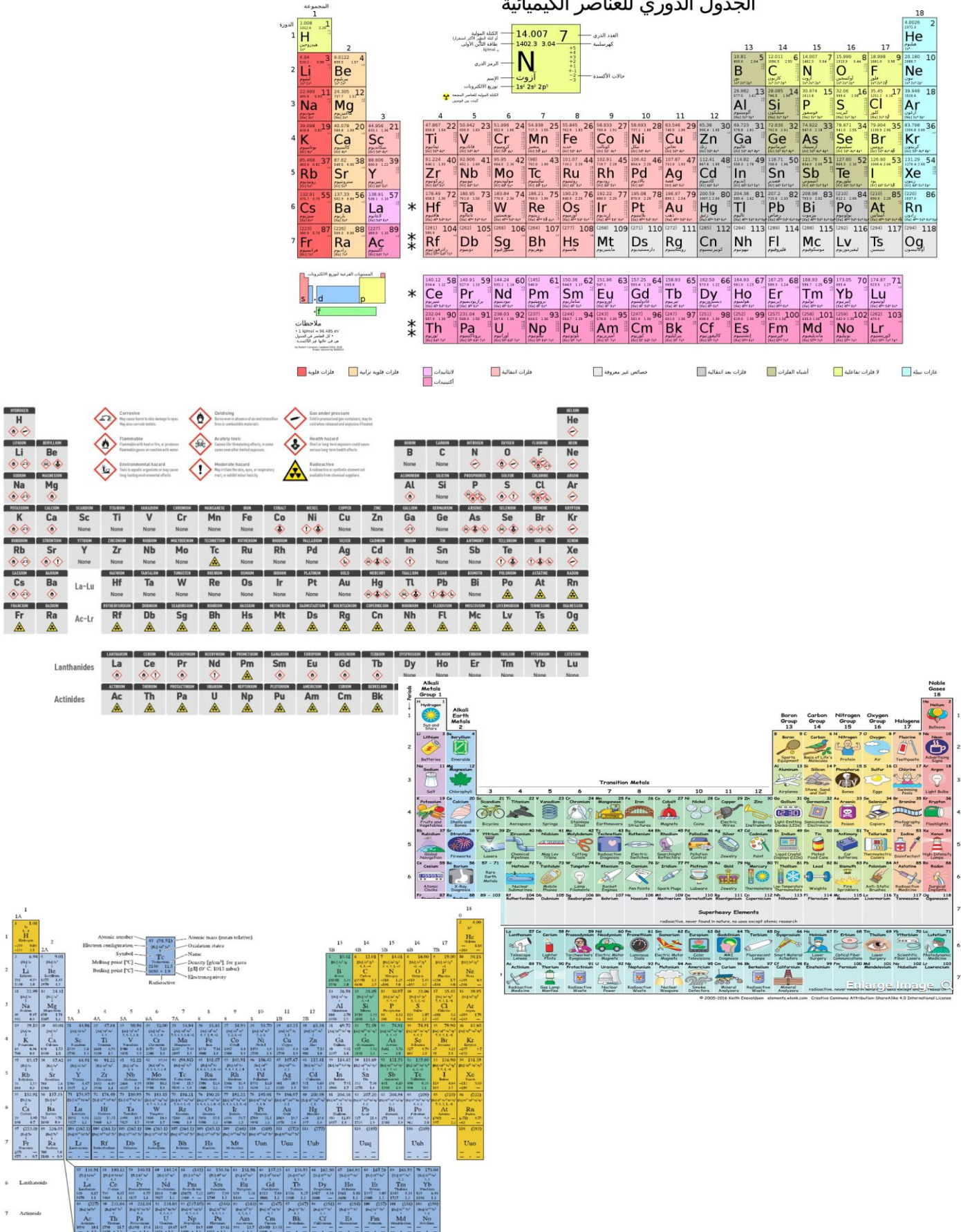
*Figure: Periodic table of elements.*

Many ceramic and semiconducting compounds, which are combinations of metallic and nonmetallic elements, have a mixture of covalent and ionic bonding. As the electronegativity difference between the atoms increases, the bonding becomes more ionic. The fraction of bonding that is covalent can be estimated from the following equation:

$$\text{Fraction covalent} = \exp(-0.25\Delta E^2)$$

where       $\Delta E$ is the difference in electronegativities.

Example below explores the nature of the bonds found in silica.

### *How Do Oxygen and Silicon Atoms Join to Form Silica?*

Assuming that silica ($SiO_2$) has 100% covalent bonding, describe how oxygen and silicon atoms in silica ($SiO_2$) are joined.

### SOLUTION

Silicon has a valence of four and shares electrons with four oxygen atoms, thus giving a total of eight electrons for each silicon atom. Oxygen has a valence of six and shares electrons with two silicon atoms, giving oxygen a total of eight electrons.
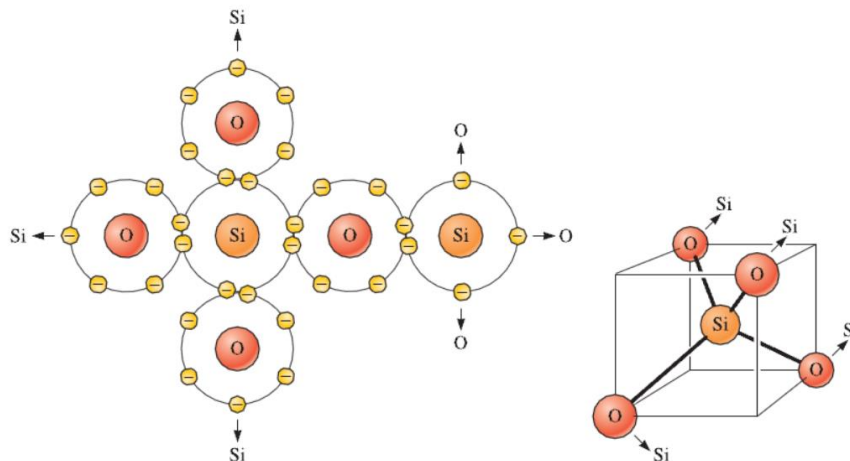


Figure: illustrates one of the possible structures. Similar to silicon (Si), a tetrahedral structure is produced.

### *Determining if Silica is Ionically or Covalently Bonded*

In a previous example, we used silica ($SiO_2$) as an example of a covalently bonded material. In reality, silica exhibits ionic and covalent bonding. What fraction of the bonding is covalent? Give examples of applications in which silica is used.

## SOLUTION

From Figure A, the electronegativity of silicon is 1.8 and that of oxygen is 3.5. The fraction of the bonding that is covalent is

$$\text{Fraction covalent} = \exp[-0.25(3.5 - 1.8)^2] = 0.486$$

Although the covalent bonding represents only about half of the bonding, the directional nature of these bonds still plays an important role in the eventual structure of $SiO_2$.

Silica has many applications. Silica is used for making glasses and optical fibers. We add nanoparticles of silica to tires to enhance the stiffness of the rubber.

High-purity silicon (Si) crystals are made by reducing silica to silicon.

### *Ionic and ionic arrangements*

The term **defect** refers to a lack of perfection in atomic or ionic order of crystals and not to any flaw or quality of an engineered material. these atomic level defects actually enable the development of formable, strong steels used in cars and buildings, aluminum alloys for aircraft, solar cells and photovoltaic modules for satellites, and many other technologies.

### *Short range order versus long rang order*

In different states of matter, we can find four types of atomic or ionic arrangements (see figure below).
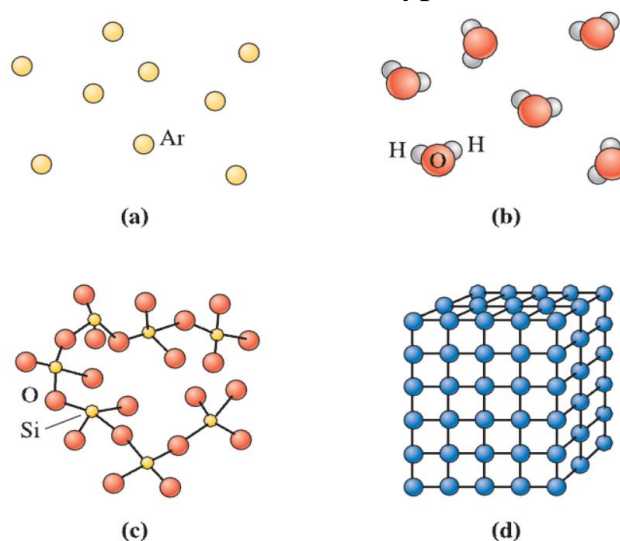


**Figure** :Levels of atomic arrangements in materials: (a) Inert monoatomic gases have no regular ordering of atoms. (b,c) Some materials, including water vapor, nitrogen gas, amorphous silicon, and silicate glass, have short-range order. (d) Metals, alloys, many ceramics and some polymers have regular ordering of atoms ions that extends through the material.

⟨10⟩

***Short-Range Order (SRO)*** A material displays short-range order (SRO) if the special arrangement of the atoms extends only to the atom's nearest neighbors.

Each water molecule in steam has short-range order due to the covalent bonds between the hydrogen and oxygen atoms; that is, each oxygen atom is joined to two hydrogen atoms, forming an angle of 104.5° between the bonds. There is no long-range order, however, because the water molecules in steam have no special arrangement with respect to each other's position.

Many polymers also display short-range atomic arrangements that closely resemble the silicate glass structure. Polyethylene is composed of chains of carbon atoms, with two hydrogen atoms attached to each carbon. Because carbon has a valence of four and the carbon and hydrogen atoms are bonded covalently, a tetrahedral structure is again produced [Figure below]. Tetrahedral units can be joined in a random manner to produce polymer chains.
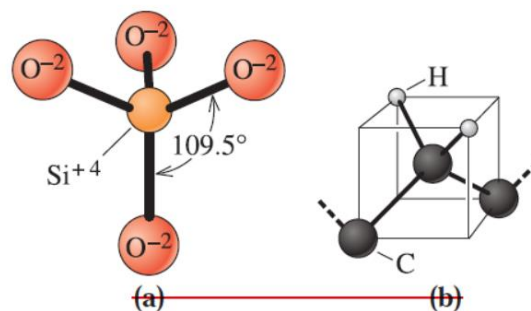


Figure : Basic Si-O tetrahedron in silicate glass. (b) Tetrahedral arrangement of C-H bonds in polyethylene.

***Long-Range Order (LRO)*** Most metals and alloys, semiconductors, ceramics, and some polymers have a crystalline structure in which the atoms or ions display **long-range order (LRO)**; the special atomic arrangement extends over much larger length scales ~ 7100 nm. The atoms or ions in these materials form a regular repetitive, grid-like pattern, in three dimensions. We refer to these materials as **crystalline materials**. If a crystalline material consists of only one large crystal, we refer to it as a *single crystal*. Single crystals are useful in many electronic and optical applications.

For example, computer chips are made from silicon in the form of large (up to 12 inch
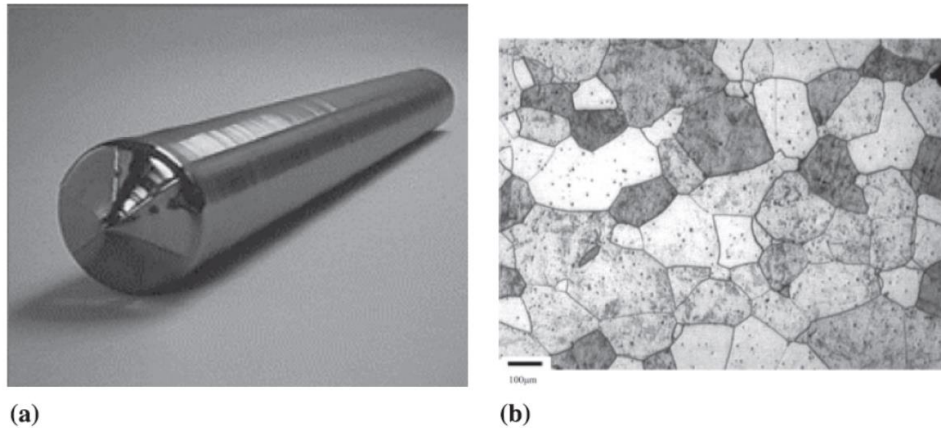
diameter) single crystals [Figure below].



**Figure**:(a) Photograph of a silicon single crystal. (b) Micrograph of a polycrystalline stainless steel showing grains and grain boundaries

Certain types of turbine blades may also be made from single crystals of nickel-based superalloys. **A polycrystalline material** is composed of many small crystals with varying orientations in space. These smaller crystals are known as **grains**. The borders between crystals, where the crystals are in misalignment, are known as **grain boundaries** Figure b above shows the microstructure of a polycrystalline stainless steel material.

Many crystalline materials we deal with in engineering applications are polycrystalline (e.g., steels used in construction, aluminum alloys for aircrafts, etc.).

**Liquid crystals** (LCs) are polymeric materials that have a special type of order. Liquid crystal polymers behave as amorphous materials (liquid-like) in one state. When an external stimulus (such as an electric field or a temperature change) is provided, some polymer molecules undergo alignment and form small regions that are crystalline, hence the name "liquid crystals." These materials have many commercial applications in liquid crystal display (LCD) technology.

## CRYSTAL STRUCTURES

**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,

**Crystal structure** of the material, the manner in which atoms, ions, or molecules are spatially arranged.
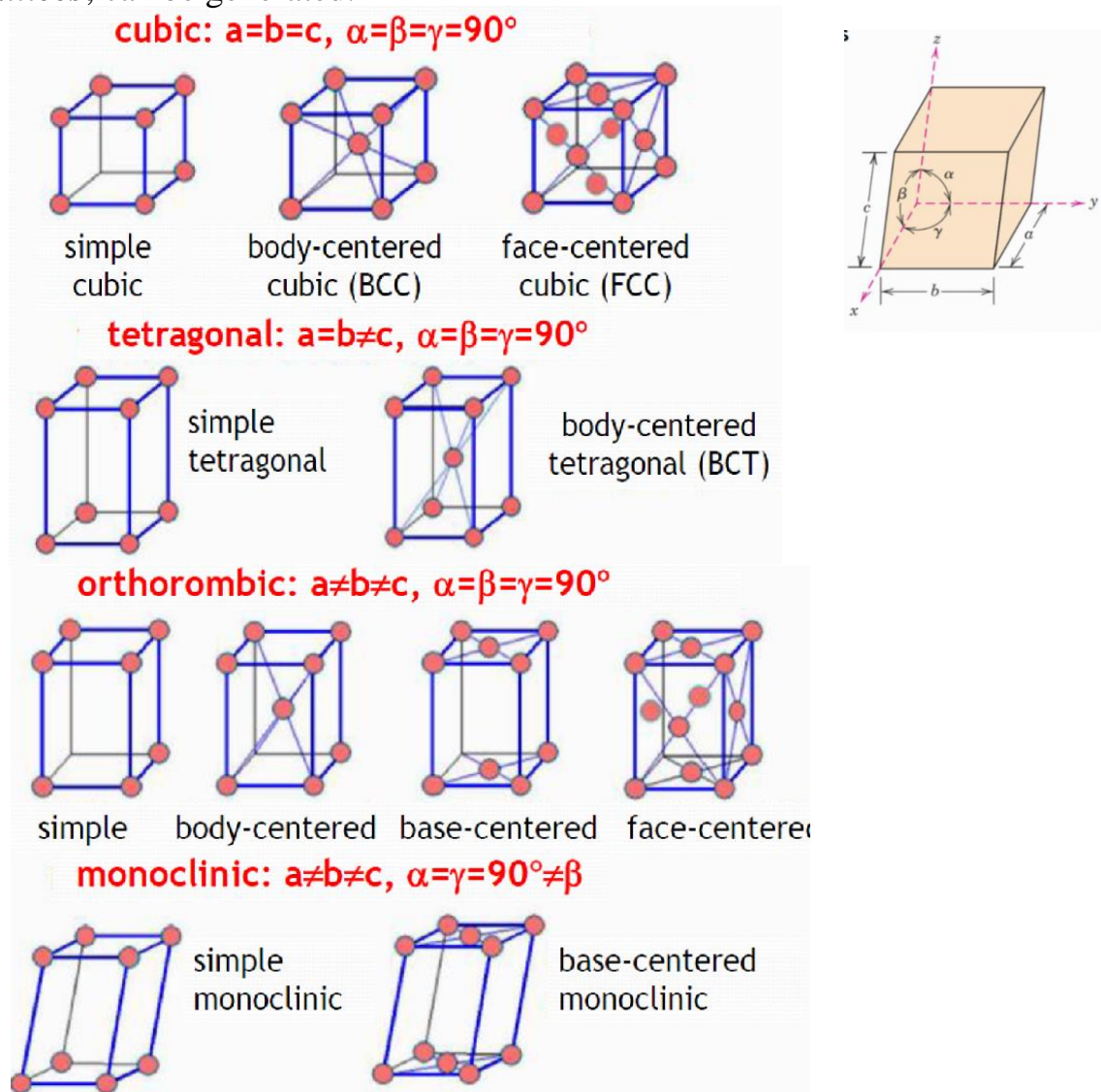
**Unit cell**:  is the basic structural unit or building block of the crystal structure and defines the crystal structure by virtue of its geometry and the atom positions within. Convenience usually dictates that parallelepiped corners coincide with centers of the hard sphere atoms. we generally use the unit cell having the highest level of geometrical symmetry.

**Non-crystalline or Amorphous** : random arrangement of atoms

*Crystal Systems*

The unit vectors *a*, *b* and *c* are called lattice parameters (Figures, below).

Based on their length equality or inequality and their orientation (the angles between them, α, β and γ) a total of 7 crystal systems (cubic, tetragonal, hexagonal, orthorhombic, rhombohedral, monoclinic, triclinic) can be defined. With the centering (face, base and body centering) added to these, 14 kinds of 3D lattices, known as *Bravais lattices*, can be generated.



cubic: a=b=c, α=β=γ=90°

simple cubic    body-centered cubic (BCC)    face-centered cubic (FCC)

tetragonal: a=b≠c, α=β=γ=90°

simple tetragonal    body-centered tetragonal (BCT)

orthorombic: a≠b≠c, α=β=γ=90°

simple    body-centered    base-centered    face-centered

monoclinic: a≠b≠c, α=γ=90°≠β

simple monoclinic    base-centered monoclinic

rhombohedral
a=b=c,
α=β=γ≠90°

hexagonal
a=b≠c,
α=β=90° γ=120°

triclinic
a≠b≠c,
α≠β≠γ≠90°

**Total of 14 Bravais lattices!**

Figure : crystal systems



F.C.C. Crystal structure:

hard-sphere unit cell
reduced-sphere unit cell
aggregate of many atoms

# simple cubic (SC) structure

- Atoms touch each other along cube edges.
- each of 8 corner atoms is shared by eight unit cells:

    8 x (1/8) = **1 atom/unit cell**

R

a = 2R
unit cell
volume = $a^3$ = $8R^3$

*BCC crystal structure*

●unit cell has cubic geometry

●atoms are located at the corners of the cube.

●Some of the materials that have a bcc structure include lithium, sodium, potassium, chromium, barium, vanadium, alpha-iron and tungsten.

●Metals which have a BCC structure are usually harder and less malleable than close-packed metals such as copper and gold.

●When the metal is deformed, the planes of atoms must slip over each other, and this is more difficult in the bcc structure.



*FCC crystal structure*

●unit cell has cubic geometry

●atoms are located at the corners and the centers of all the cube faces.

●familiar metals with FCC crystal structure copper aluminium silver gold

## FCC crystal structure

each of 8 corner atoms is shared by eight unit cells;
each of 6 face-centered atoms belongs to only two.
8 x (1/8) + 6 x (1/2) = 1 + 3 = **4 atoms/unit cell**

The volume of the unit cell,

$$a^3 = (2R\sqrt{2})^3 = 16R^3\sqrt{2}$$
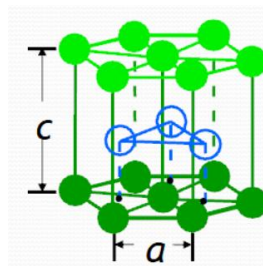
$4R = \sqrt{2}.a$
$(a = 2R\sqrt{2})$

*Hexagonal close packed (HCP) crystal structure*

●The HCP metals: Cd, Mg, Ti, and Zn.

●top and bottom faces consist of six atoms that form regular hexagons and surround a single atom in the center.

●Another plane that provides three additional atoms to the unit cell is situated between the top and bottom planes. The atoms in this mid-plane have as nearest neighbors atoms in both of the adjacent two planes.

●The equivalent of **six atoms** is contained in each unit cell

●one-sixth of each of the 12 top and bottom face corner atoms, one-half of each of the 2 center face atoms, and all 3 midplane interior atoms.:

**12 x 1/6 + 2 x ½ +   3 =    2 +1   + 3 = 6**
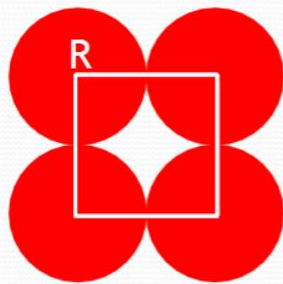
**corner       face    midplane**

# simple cubic (SC) structure

- Atoms touch each other along cube edges.
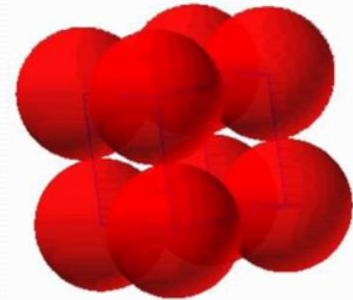- each of 8 corner atoms is shared by eight unit cells:

  8 x (1/8) = **1 atom/unit cell**

R

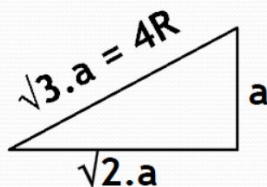a = 2R
unit cell
volume = a³ = 8R³

*BCC crystal structure*

●unit cell has cubic geometry

●atoms are located at the corners of the cube.

●Some of the materials that have a bcc structure include lithium, sodium, potassium, chromium, barium, vanadium, alpha-iron and tungsten.

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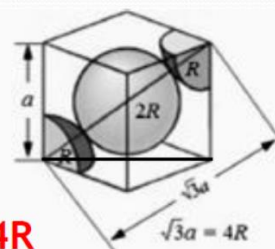
# body centred cubic (BCC) structure

- Atoms touch each other along cube diagonals.
- each of 8 corner atoms is shared by eight unit cells; single center atom is wholly owned:

  8 x (1/8) + 1 = 1 + 1 = **2 atoms/unit cell**

- each center atom touches eight corner atoms:

  **8 nearest neighbors**

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

a

$\sqrt{2}.a$

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

a

2R

R

$\sqrt{3}a$

$\sqrt{3}a = 4R$

〈17〉

*FCC crystal structure*

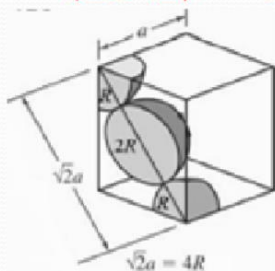●unit cell has cubic geometry

●atoms are located at the corners and the centers of all the cube faces.

●familiar metals with FCC crystal structure copper aluminium silver gold

## FCC crystal structure

each of 8 corner atoms is shared by eight unit cells;
each of 6 face-centered atoms belongs to only two.
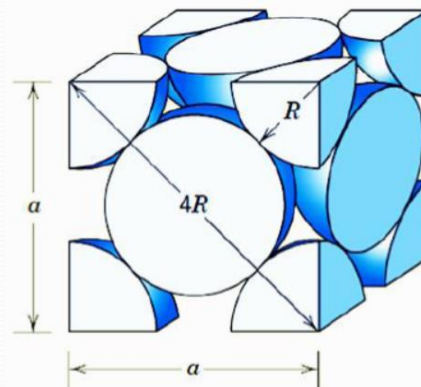8 x (1/8) + 6 x (1/2) = 1 + 3 = **4 atoms/unit cell**

The volume of the unit cell,

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4R=√2.a
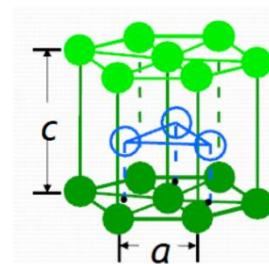(a = 2R√2)

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**12 x 1/6 + 2 x ½ +   3 =    2 +1   + 3 = 6**
**corner       face   midplane**

## Atomic packing factor

Atomic packing factor (APF) or packing efficiency indicates how closely atoms are packed in a unit cell and is given by the ratio of volume of atoms in the unit cell and volume of the unit cell.

$$APF = \frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}} = \frac{V_S}{V_C}$$

## Atomic packing factor (FCC lattice)

In the FCC unit cell effective number of atoms = 8 corner atoms x (1/8) (each atom is shared by 8 unit cells) + 6 face centered atoms x1/2 (each shared by two unit cells) = 4 atoms. Considering the atoms as hard spheres of radius $R$.
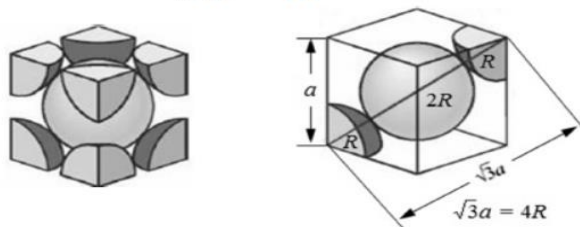The relation between $R$ and the FCC cell side $a$ as shown in the figure below is     $\sqrt{2}a = 4R$
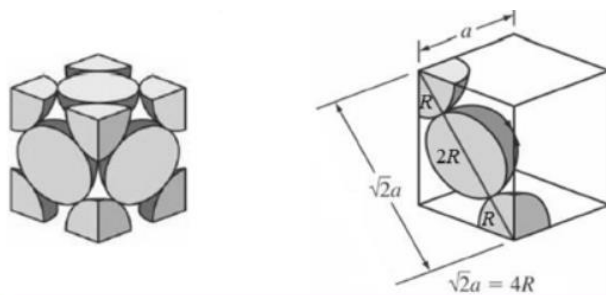


$$APF(FCC) = \frac{4 \times \frac{4}{3}\pi R^3}{a^3} = \frac{16 \times 2\sqrt{2}\pi\, a^3}{3 \times 64a^3} = 0.74$$

## Atomic packing factor(BCC lattice)

For BCC crystals effective number of atoms per unit cell is 8 x 1/8 + 1 = 2 and the relation between R and a is   $\sqrt{3}a = 4R$
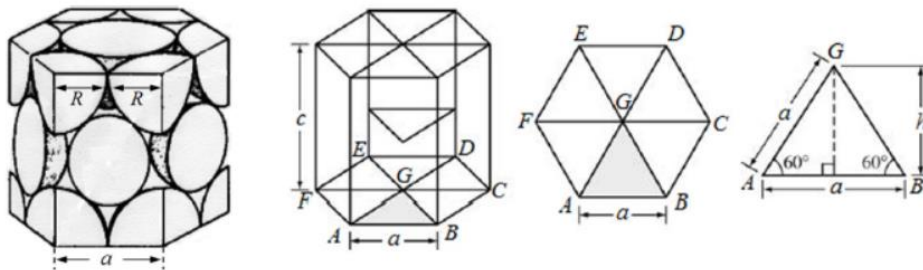


$$APF(BCC) = \frac{2 \times \frac{4}{3}\pi R^3}{a^3} = \frac{8 \times 3\sqrt{3}\pi\, a^3}{3 \times 64a^3} = 0.68$$

### Atomic packing factor(HCP lattice)

In the Hexagonal unit cell, number of atoms = 12 corner atoms x 1/6 (shared by six unit cells) + Two face atoms x 1/2 + 3 interior = 6.

$$2R = a$$

Unit cell volume = (6 x ½ x a x h) x c = (3 x a x a sin60°) x c
= $3a^2 c \sin 60°$

$$APF(HCP) = \frac{6 \times \frac{4}{3}\pi R^3}{3a^2 c \sin 60°} = \frac{8\pi a^3}{3 \times 8 \times 1.414 a^3} = 0.74$$

### Point Coordinates

Position of any point in a unit cell is given by its coordinates or distances from the x, y and z axes in terms of the lattice vectors a, b and c.

Thus the point located at a/2 along x axis, b/3 along y axis and c/2 along z axis, as shown in the figure below, has the coordinates $\frac{1}{2}\frac{1}{3}\frac{1}{2}$
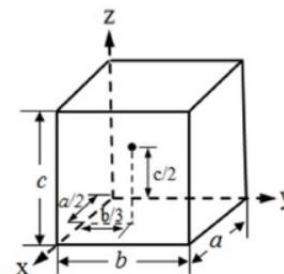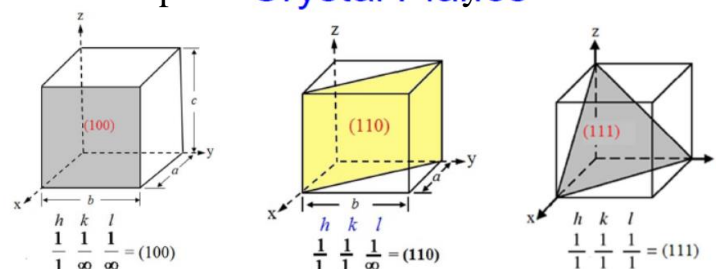
### Miller Indices

Planes in a crystal are described by notations called Miller indices

-Miller indices of a plane, indicated by h k l, are given by the reciprocal of the intercepts of the plane on the three axes.

-The plane, which intersects X axis at 1 (one lattice parameter) and is parallel to Y and Z axes, has Miller indices

h = 1/1 = 1, k = 1/∞ = 0, l = 1/∞ = 0. It is written as (hkl) = (100).

-Miller indices of some other planes in the cubic system are shown in the figures below

| h | k | l | |
|---|---|---|---|
| $\frac{1}{1}$ | $\frac{1}{\infty}$ | $\frac{1}{\infty}$ | = (100) |

| h | k | l | |
|---|---|---|---|
| $\frac{1}{1}$ | $\frac{1}{1}$ | $\frac{1}{\infty}$ | = (110) |

| h | k | l | |
|---|---|---|---|
| $\frac{1}{1}$ | $\frac{1}{1}$ | $\frac{1}{1}$ | = (111) |

*To find the Miller Indices of a plane, follow these steps:*
1-Determine the intercepts of the plane along the crystal axes
2-Take the reciprocals
3-Clear fractions
4-Reduce to lowest terms and enclose in brackets ( )
Example: Intercepts on a, b, c : ¾, ½, ¼ (h k l) = (4/3, 2, 4) = (2 3 6)

*Crystal Planes*
Planes can also have negative intercept e.g. 1, -1/2, 1    h k l = 1 -2 1. This is denoted
as ( 1 $\overline{2}$ 1 )
*Family of planes {hkl}*
Planes having similar indices are equivalent, e.g. faces of the cube (100), (010) and
(001). This is termed as a family of planes and denoted as {100} which includes all
the (100) combinations including negative indices.
Some other equivalent planes are shown in the next slide.
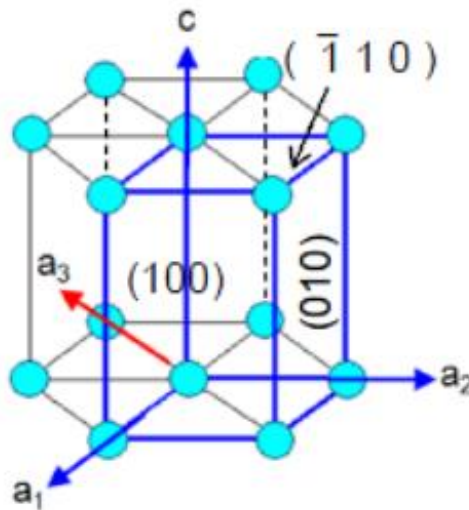
Equivalent Planes
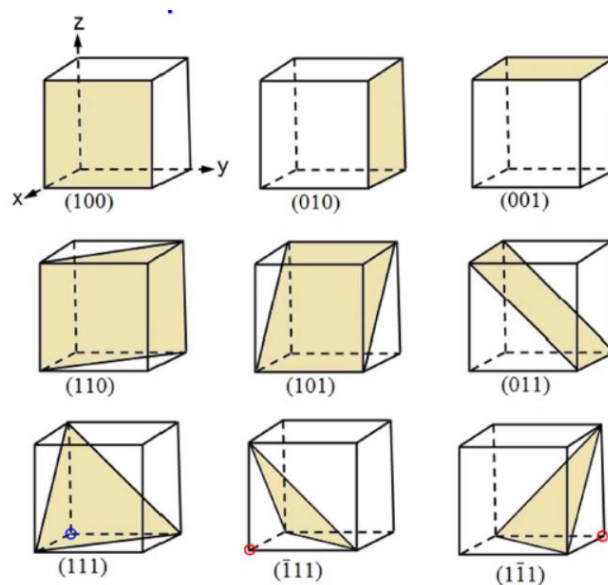


Note the shift of origin from blue to red circle for the negative indices
Planes in Hexagonal system
-In the cubic system all the faces of the cube are equivalent,
that is, they have similar indices.
In order to address this, a fourth axis (a3) which is opposite to the vector sum of a1
and a2 is used and a corresponding fourth index *i* is used along with *hkl*. Therefore
the indices of a plane is given by *(hkil)* where *i = -(h+k)*. Sometime *i* is replaced with
a dot and written as (h k . l)

-However, this is not the case in the hexagonal system. The six prism faces for example have indices (1 0 0), (0 1 0), ($\bar{1}$ 1 0 ), ($\bar{1}$ 0 0 ), (0$\bar{1}$ 0), (1$\bar{1}$ 0 ), which are not same.



The indices of six faces now become (1 0$\bar{1}$ 0), (0 1$\bar{1}$ 0), ($\bar{1}$ 1 0 0), ($\bar{1}$ 0 1 0), (0$\bar{1}$ 1 0), (1$\bar{1}$ 0 0 ) which are now equivalent and belong to the {1 0$\bar{1}$ 0 } family of planes.
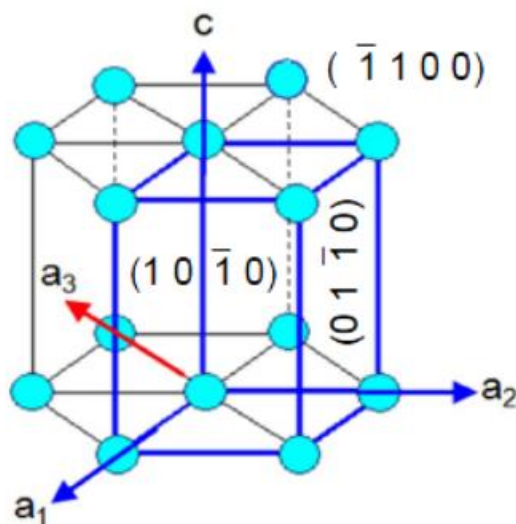
### *Lattice Positions and Directions:*

1) Always establish an origin

2) Determine the coordinates of the lattice

points of interest

3) Translate the vector to the origin if

required by drawing a parallel line or move the origin.

4) Subtract the second point from the first: u2-u1,v2-v1,w2-w1

5) Clear fractions and reduce to lowest terms

6) Write direction with square brackets [uvw]

7) Negative directions get a hat.
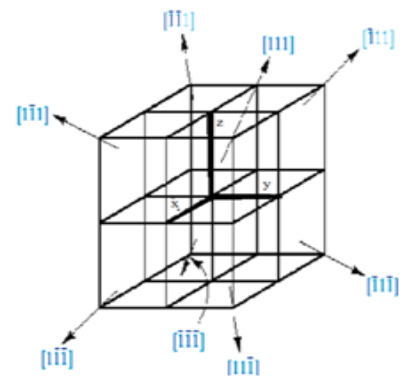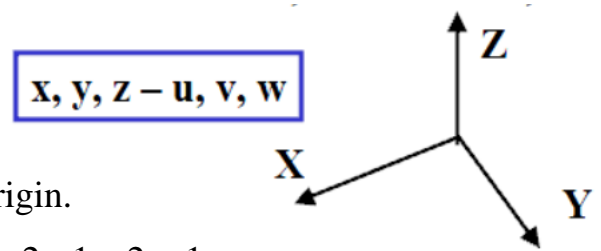
### **Remember Terminology:**

•Defined coordinate system: x, y, z

•Respective unit cell edge lengths: a, b, c

•Direction: Denoted by [uvw]

•Family of direction(s): Denoted by: <uvw>

•Plane: Denoted by: (hkl)

•Family of Plane(s): Denoted by: {hkl}

•Directions are always perpendicular to their respective planes, i.e. [111] perpendicular (111) (for cubic systems)

•Families of equivalent planes are equal with respect to symmetrical structures, they do not have to be parallel. Equivalent planes must be translated to the correct atomic positions in order to maintain the proper crystal symmetry.

• Families of directions are equivalent in absolute magnitude.

• (222) planes are parallel to the (111) planes but not equal.

• Intercepts for the (222) planes are 1/2,1/2,1/2

• Intercepts for the (333) planes are 1/3,1/3,1/3, remember this is in what we call "reciprocal space". If you draw out the (333) plane it is parallel to the (111) plane but not equivalent.

(23)
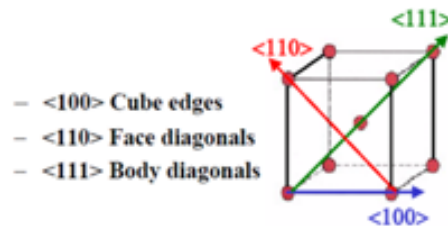
### Density Computations

Since the entire crystal can be generated by the repetition of the unit cell, the density of a crystalline material, $\rho$ = the density of the unit cell = (atoms in the unit cell, n )

× (mass of an atom, M) / (the volume of the cell, Vc)

Atoms in the unit cell, n = 2 (BCC); 4 (FCC); 6 (HCP)

Mass of an atom, M = Atomic weight, A, in amu (or g/mol) is given in the periodic table. To translate mass from amu to grams we have to divide the atomic weight in amu by the Avogadro number NA = 6.023 × $10^{23}$ atoms/mol

The volume of the cell, Vc = a3 (FCC and BCC) a = 2R$\sqrt{2}$ (FCC); a = 4R/$\sqrt{3}$ (BCC)

where R is the atomic radius.

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

### Polycrystalline Materials

• In polycrystalline materials, grain orientations are random, so bulk material properties are isotropic.

• Some polycrystalline materials have grains with preferred orientations (texture), so properties are dominated by those relevant to the texture orientation.

### Polymorphism and Allotropy

Some materials may exist in more than one crystal structure, this is called **polymorphism**. If the material is an elemental solid, it is called allotropy.

An example of allotropy is carbon, which can exist as diamond, graphite, and amorphous carbon.

Diamod     Graphite     Buckminsterflurene

Carbon nanotube