



# ICT 1107: Physics

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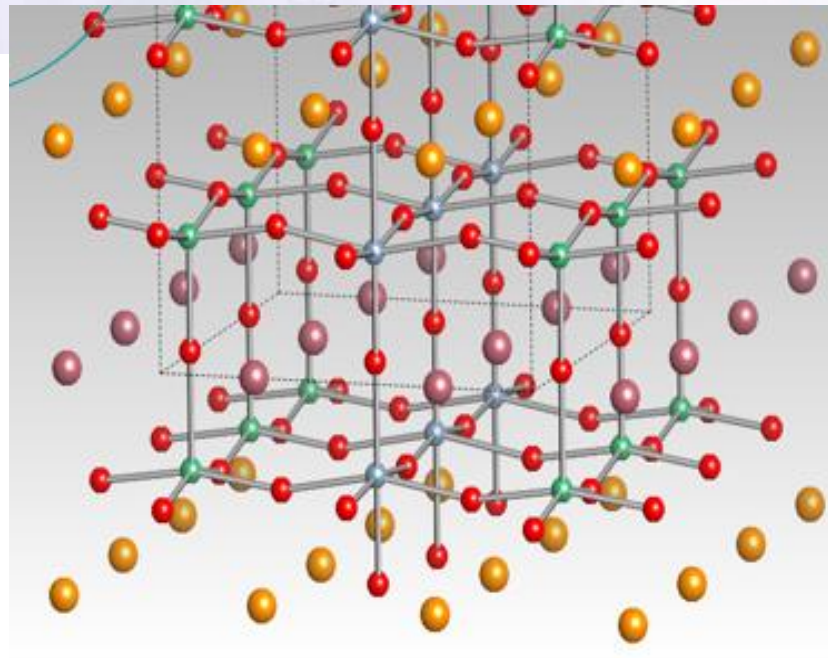
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# ICT 1107: Physics

## 3. Structure of Matters

Crystalline and non-crystalline solids, single crystal and polycrystal solids, unit cell, crystal systems, co-ordinations number, crystal planes and directions, sodium chloride and CsCl structure, packing factor, Miller indices, relation between interplanar spacing and Miller indices, Bragg's Law, methods of determination of interplanar spacing from diffraction patterns: Defects in solids: point defects, line defects; Bonds in solids, inter-atomic distances, calculation of cohesive and bonding energy; Introduction to band theory; distinction between metal, semiconductor and insulator.





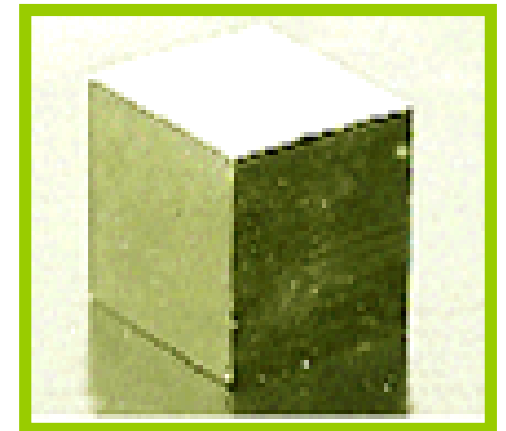
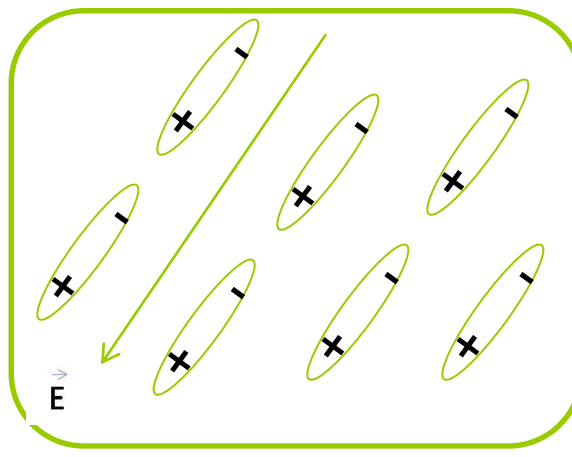
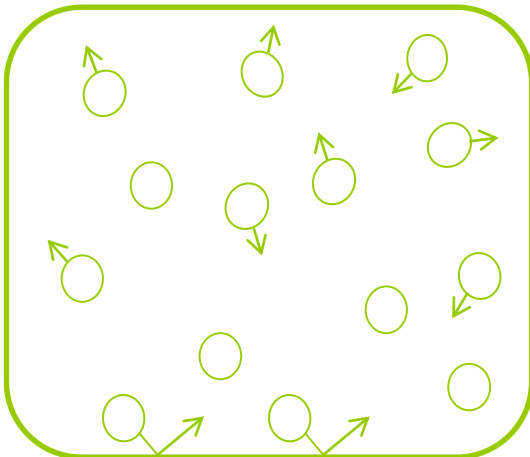
# Basics of Solid State Physics

**MATTER**

**GASES**

**LIQUIDS  
AND LIQUID  
CRYSTALS**

**SOLIDS**



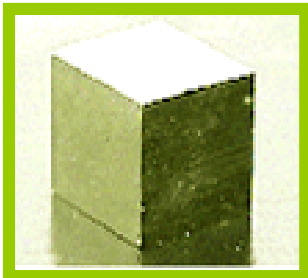


# Classification of Solids

## SOLID MATERIALS

**CRYSTALLINE**

**Single Crystal**



**POLYCRYSTALLINE**



**AMORPHOUS  
(NON-CRYSTALLINE)**





# Basics of Solid State Physics

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- ❑ Explains the properties of solid materials.
- ❑ Explains the properties of a collection of atomic nuclei and electrons interacting with electrostatic forces.
- ❑ Formulates fundamental laws that govern the behaviour of solids.



# Crystalline Solids

- ❑ Crystalline materials are solids with an **atomic structure based on a regular repeated pattern.**
- ❑ The majority of all solids are crystalline.
- ❑ More progress has been made in understanding the behaviour of crystalline solids than that of non-crystalline materials **since the calculation are easier** in crystalline materials.
- ❑ **Understanding the electrical properties of solids** is right at the heart of modern society and technology.



# Crystal Structure

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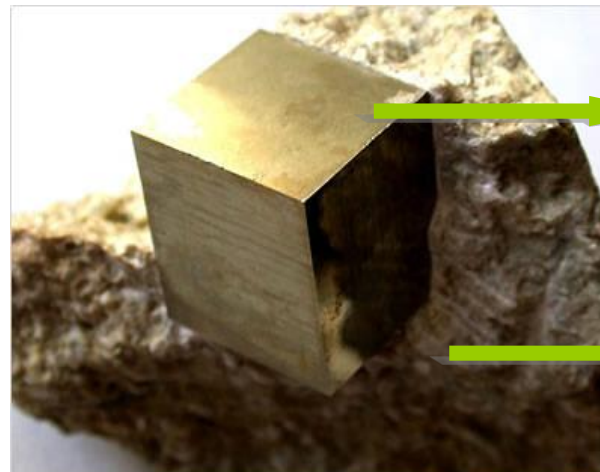
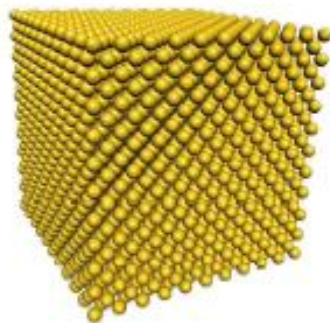
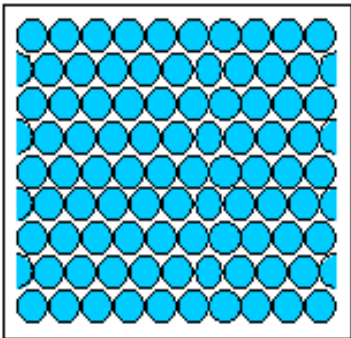
- Elementary Crystallography
  - ✓ Solid materials (crystalline, polycrystalline, amorphous)
  - ✓ Crystallography
  - ✓ Crystal Lattice
  - ✓ Crystal Structure
  - ✓ Types of Lattices
  - ✓ Unit Cell
  
- Typical Crystal Structures  
(14 Bravais Lattices and the Seven Crystal System)





# Single Crystals

- **Single crystals** have a periodic atomic structure across its whole volume.
- At long range length scales, each atom is related to every other equivalent atom in the structure by translational or rotational symmetry



Single Pyrite Crystal

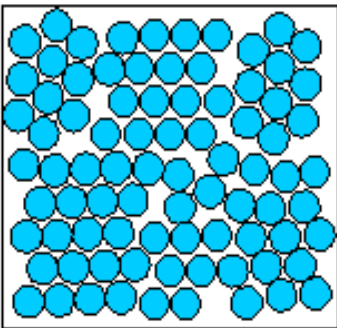
Amorphous Solid



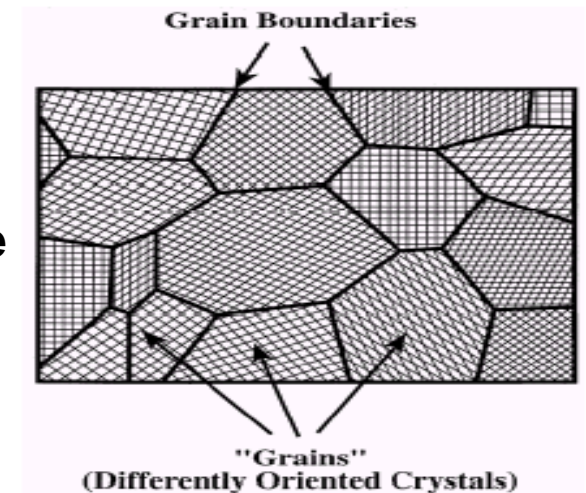


# Polycrystalline Solids

- **Polycrystalline materials** are made up of an aggregate of *many small single crystals* (also called crystallites or grains).
- **Polycrystalline materials** have a high degree of order over many atomic or molecular dimensions.
- **Grains (domains)** are separated by **grain boundaries**. The atomic order can vary from one domain to the next.
- The grains are usually **100 nm - 100 microns in diameter**.
- Polycrystals with grains less than 10 nm in diameter are **nanocrystalline**



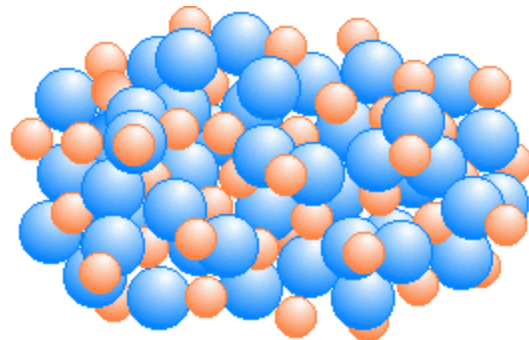
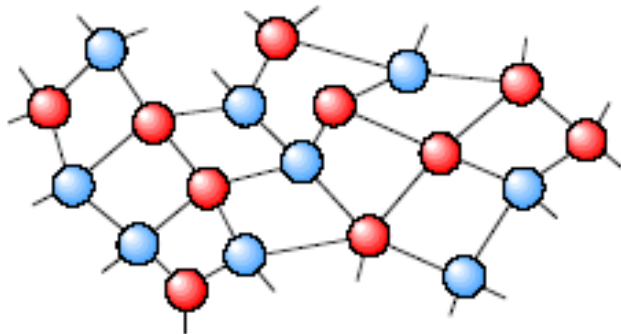
Polycrystalline  
Pyrite form  
(Grain)





# Amorphous Solids

- ❑ **Amorphous (Non-crystalline) Solids** are made up of randomly orientated atoms, ions, or molecules that do not form defined patterns or lattice structures.
- ❑ Amorphous materials have order only within a few atomic or molecular dimensions.
- ❑ Amorphous materials do not have any long-range order, but they have varying degrees of short-range order.
- ❑ Examples to amorphous materials include amorphous silicon, plastics, and glasses.
- ❑ Amorphous silicon can be used in solar cells and thin film transistors.





# Crystallography

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- ✓ Crystallography is a branch of science that deals with the geometric description of crystals and their internal atomic arrangement.
- ✓ It's important the symmetry of a crystal because it has a profound influence on its properties.
- ✓ Structures should be classified into different types according to the symmetries they possess.
- ✓ Energy bands can be calculated when the structure has been determined.



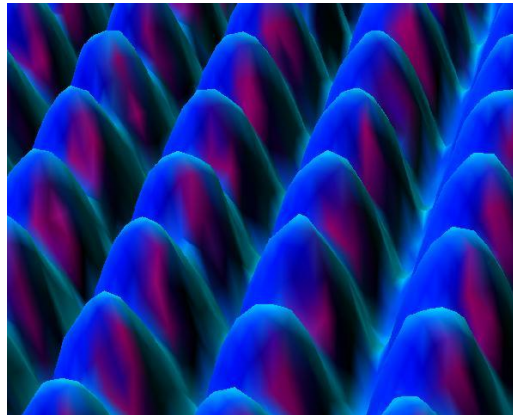
# Crystal Lattice

## What is a crystal lattice?

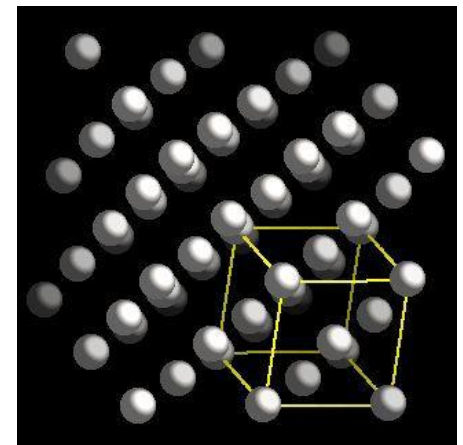
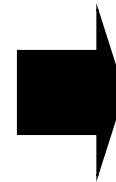
In crystallography, only the geometrical properties of the crystal are of interest, therefore one replaces each atom by a geometrical point located at the equilibrium position of that atom.



Platinum



Platinum surface  
(scanning tunneling microscope)

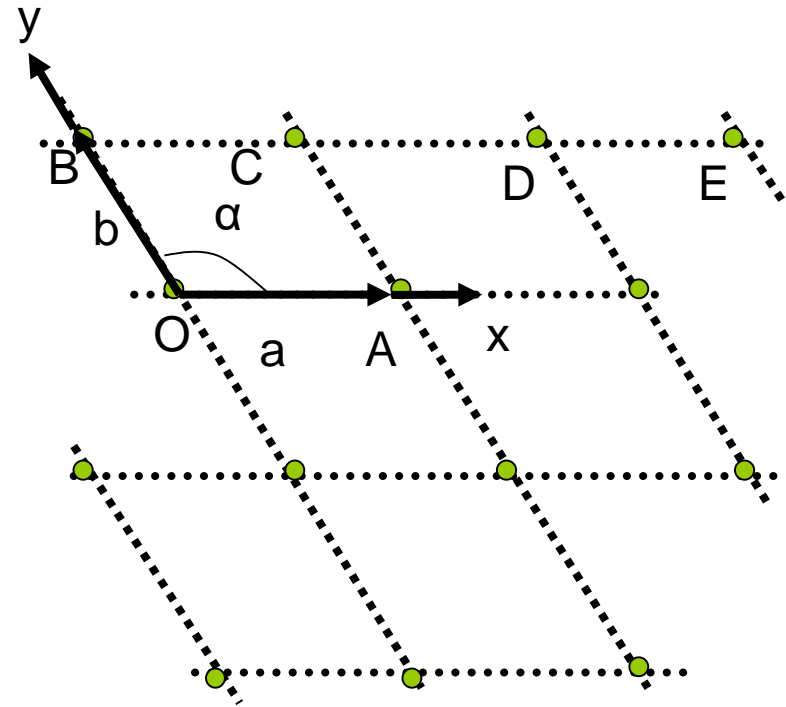


Crystal lattice and  
structure of Platinum<sup>12</sup>



# Crystal Lattice

- ✓ An infinite array of points in space,
- ✓ Each point has identical surroundings to all others
- ✓ Arrays are arranged in a periodic manner.

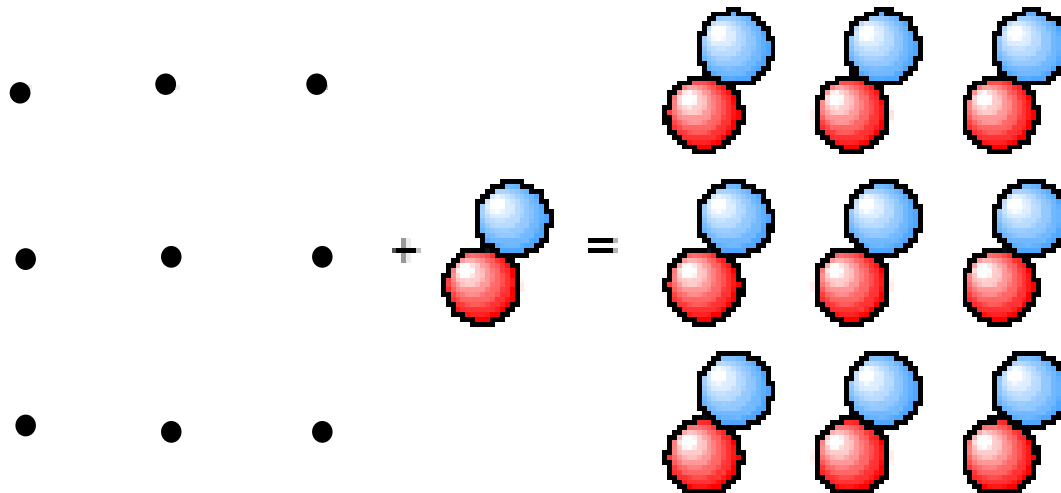




# Crystal Structure

- Crystal structures can be obtained by attaching atoms, groups of atoms or molecules which are called basis (motif) to the lattice sites of the lattice point.

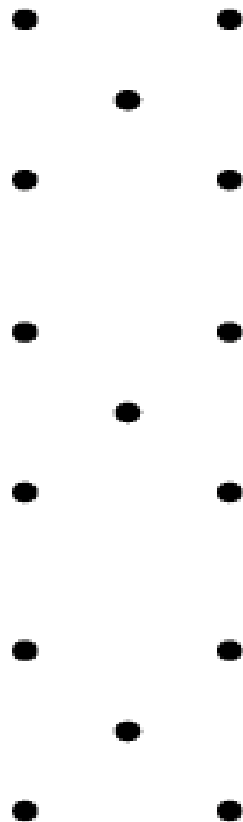
**Crystal Structure = Crystal Lattice + Basis**





# 2D Bravais Lattice with different basis choices

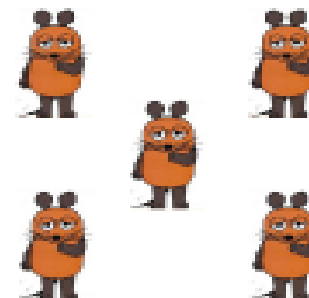
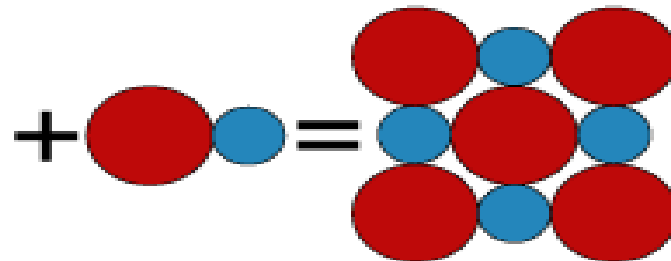
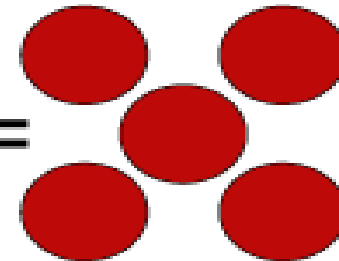
Bravais  
lattice



basis



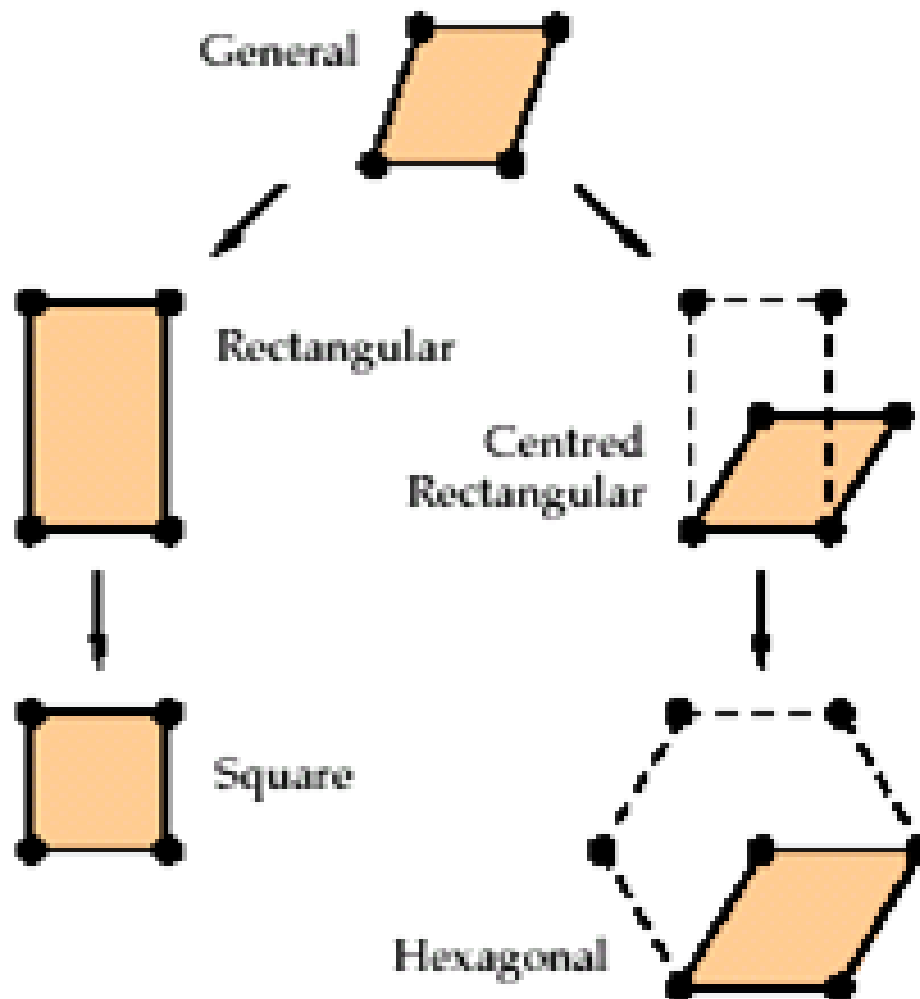
crystal







# 2D Bravais Lattice Types



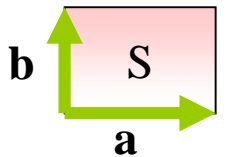


# 2D Unit Cell

- The smallest component of the crystal (group of atoms, ions or molecules), which when stacked together with pure translational repetition reproduces the whole crystal.

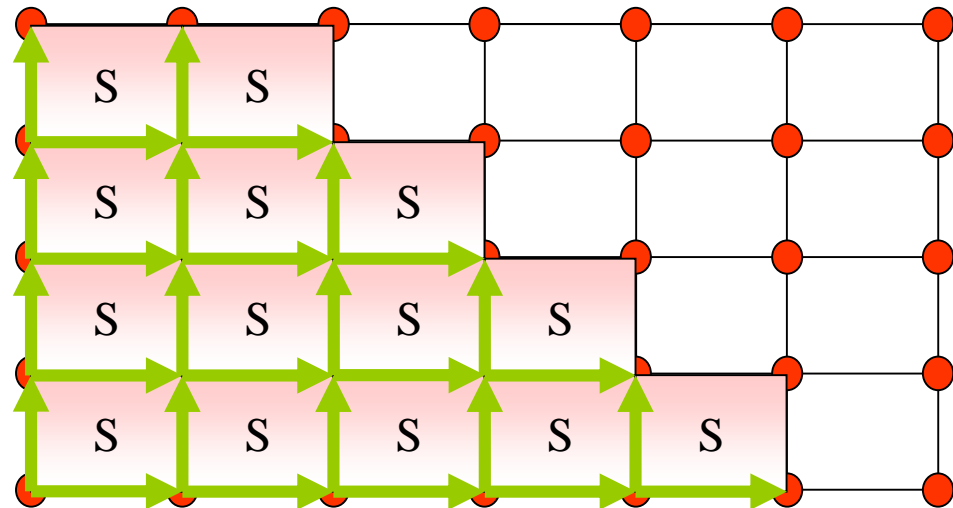
OR,

The unit cell is the building block for the crystal structure. Repetition of the unit cell generates the entire crystal.

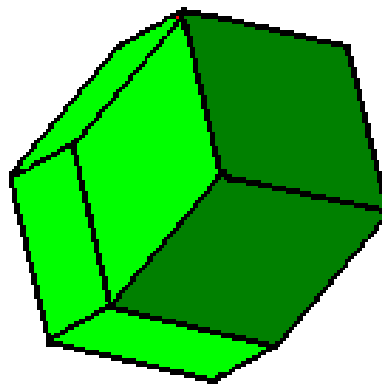
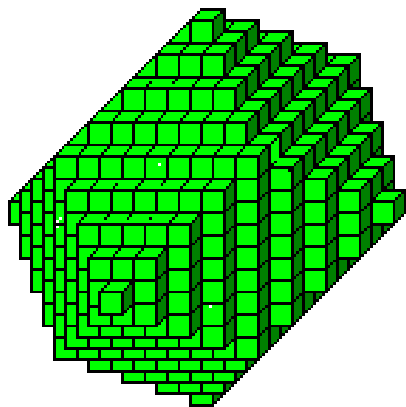
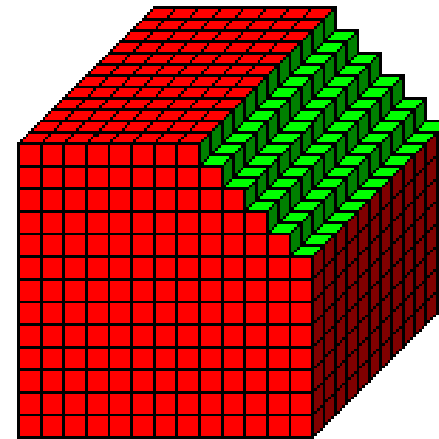
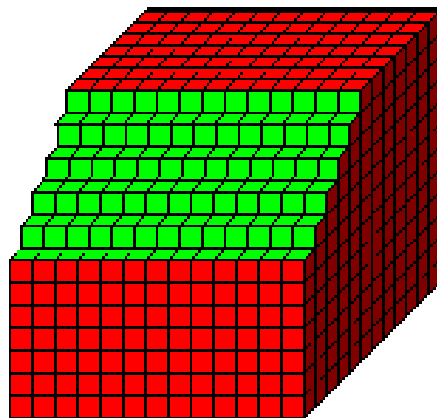
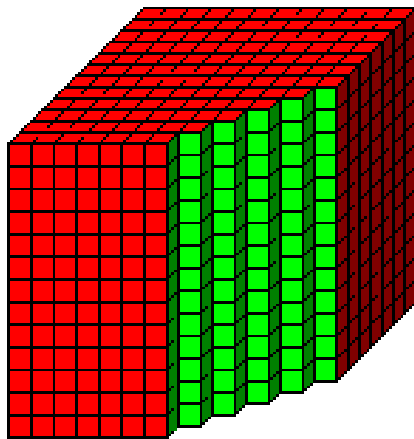


**Unit Cell**

2D-Crystal

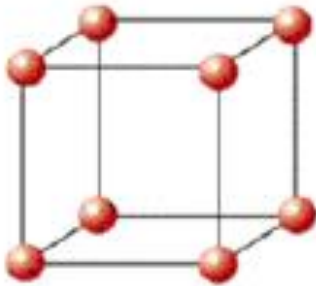


# 3D Unit Cell

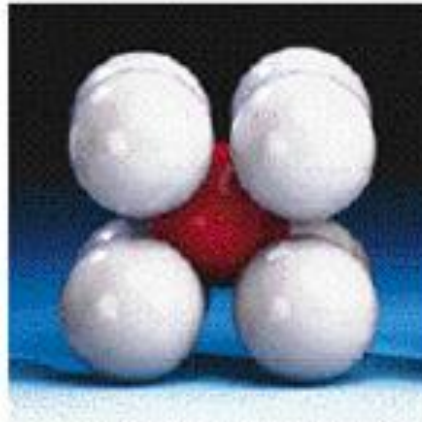
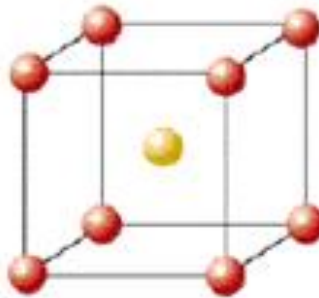




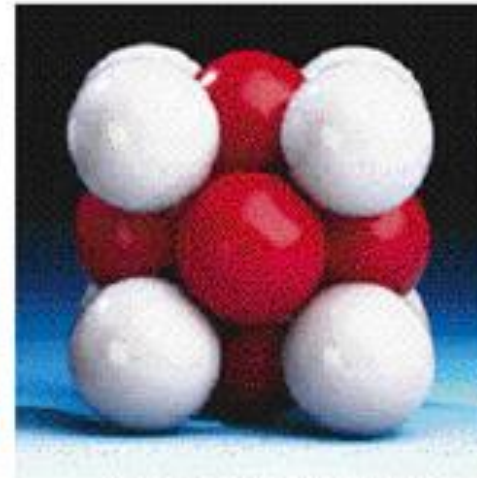
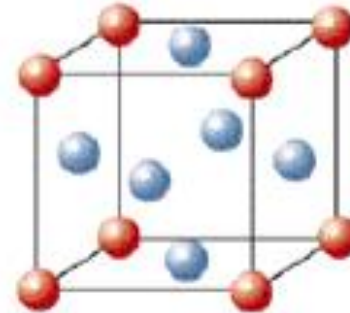
# 3 Common 3D Unit Cells



simple cubic



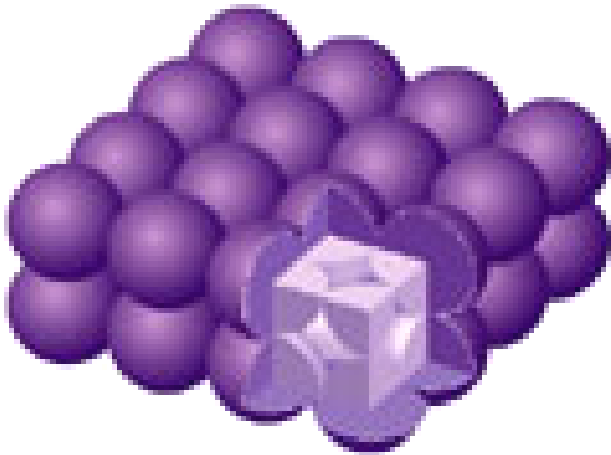
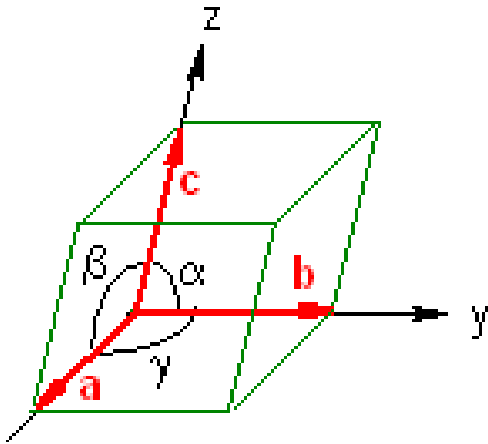
body-centered cubic



face-centered cubic



# Unit Cell



- The unit cell and, consequently, the entire lattice, is uniquely determined by the six lattice constants:  $a$ ,  $b$ ,  $c$ ,  $\alpha$ ,  $\beta$  and  $\gamma$ .
- Only  $1/8$  of each lattice point in a unit cell can actually be assigned to that cell.
- Each unit cell in the figure can be associated with  $8 \times 1/8 = 1$  lattice point.



# 3D Crystal Structures

## 14 Bravais Lattice & 7 Crystal System

- Cubic Crystal System (SC, BCC, FCC)
- Hexagonal Crystal System (S)
- Triclinic Crystal System (S)
- Monoclinic Crystal System (S, Base-C)
- Orthorhombic Crystal System (S, Base-C, BC, FC)
- Tetragonal Crystal System (S, BC)
- Trigonal (Rhombohedral) Crystal System (S)

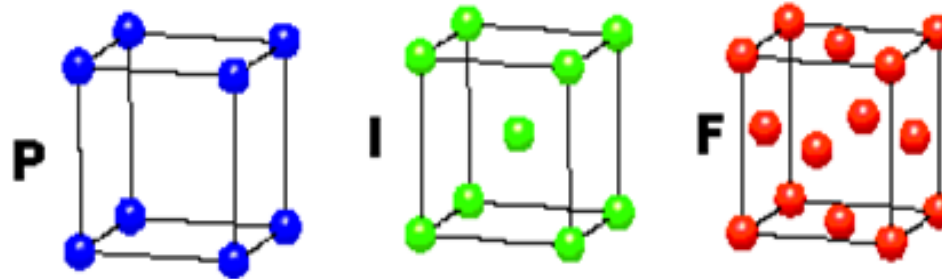


# 14 Bravais Lattice & 7 Crystal System

## CUBIC

$$a = b = c$$

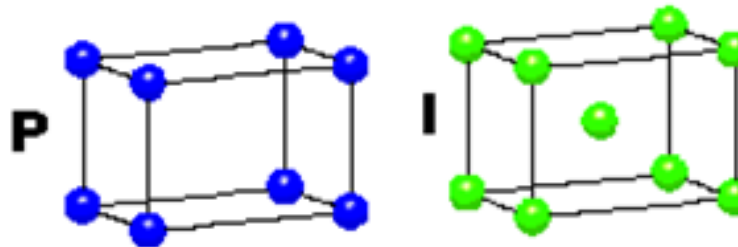
$$\alpha = \beta = \gamma = 90^\circ$$



## TETRAGONAL

$$a = b \neq c$$

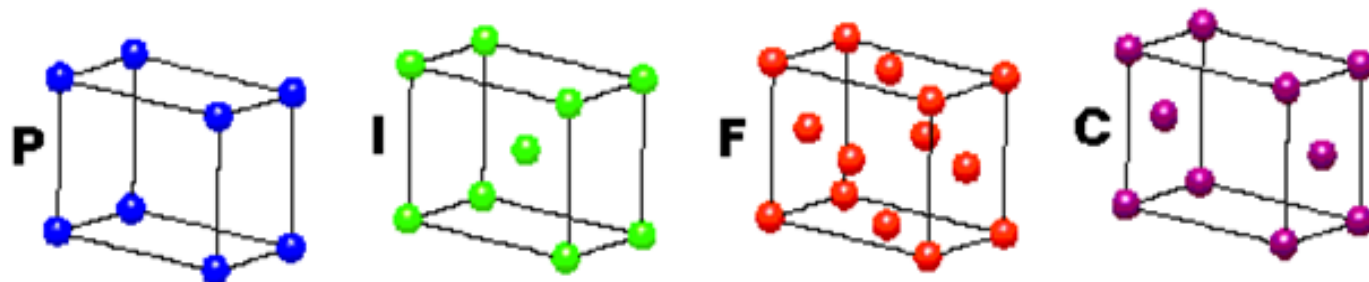
$$\alpha = \beta = \gamma = 90^\circ$$



## ORTHORHOMBIC

$$a \neq b \neq c$$

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







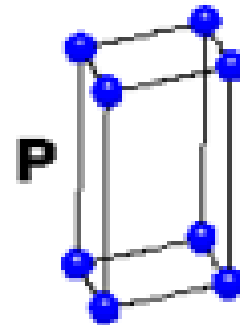
# 14 Bravais Lattice & 7 Crystal System

## HEXAGONAL

$$a = b \neq c$$

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

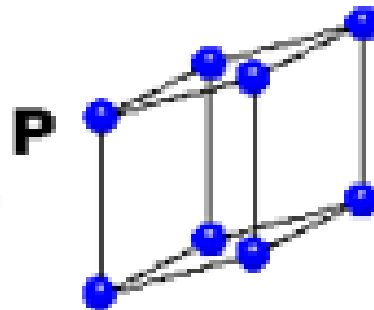
$$\gamma = 120^\circ$$



## TRIGONAL

$$a = b = c$$

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

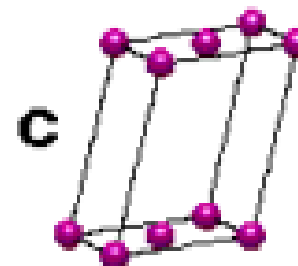
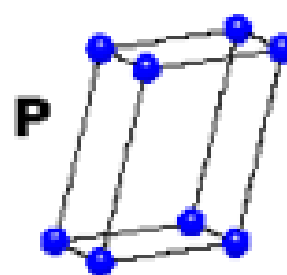


## MONOCLINIC

$$a \neq b \neq c$$

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

$$\beta \neq 120^\circ$$



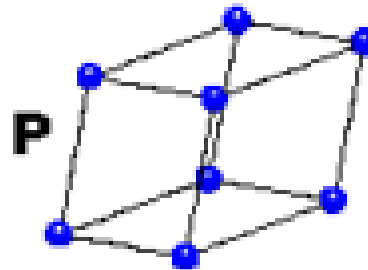


# 14 Bravais Lattice & 7 Crystal System

## TRICLINIC

$$a \neq b \neq c$$

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



### 4 Types of Unit Cell

P = Primitive

I = Body-Centred

F = Face-Centred

C = Side-Centred

+

7 Crystal Classes

→ 14 Bravais Lattices



# Summary: Crystal Systems

## Cubic system

- 3 mutually  $\perp$  axes;  $\alpha = \beta = \gamma = 90$
- 3 equal edges;  $a = b = c$  (lattice constants)

**Cubic system is only one of seven crystal systems!**

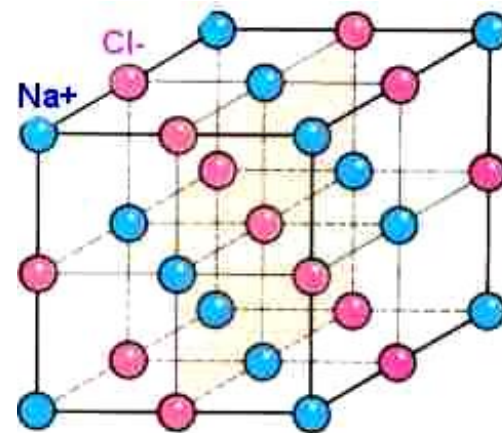
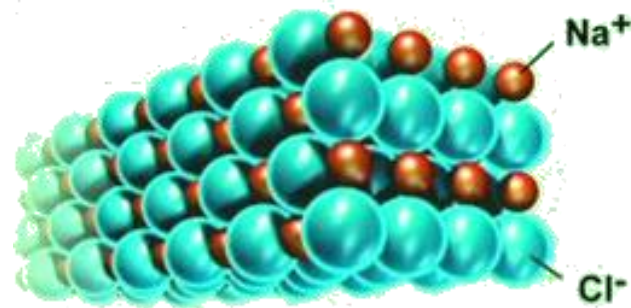
(3) Cubic	$a = b = c$	All angles = 90
(2) Tetragonal	$a = b \neq c$	All angles = 90
(4) Orthorhombic	$a \neq b \neq c$	All angles = 90
(2) Monoclinic	$a \neq b \neq c$	2 angles = 90; one $\neq 90$
(1) Triclinic	$a \neq b \neq c$	All angles $\neq$ ; none = 90
(1) Hexagonal	$a = b \neq c$	2 Angles = 90; one = 120
(1) Rhombohedral	$a = b = c$	All angles equal $\neq 90$

Seven crystal systems are results from the arrangement of 14 different ways of arranging equivalent points in space – Bravais lattices



# Structure of NaCl

- ❖ Sodium chloride crystallizes in a cubic lattice, but with a different unit cell.
- ❖ Sodium chloride structure consists of equal numbers of sodium and chlorine ions placed at alternate points of a simple cubic lattice.
- ❖ Each ion has six of the other kind of ions as its nearest neighbours.





# Interatomic Forces

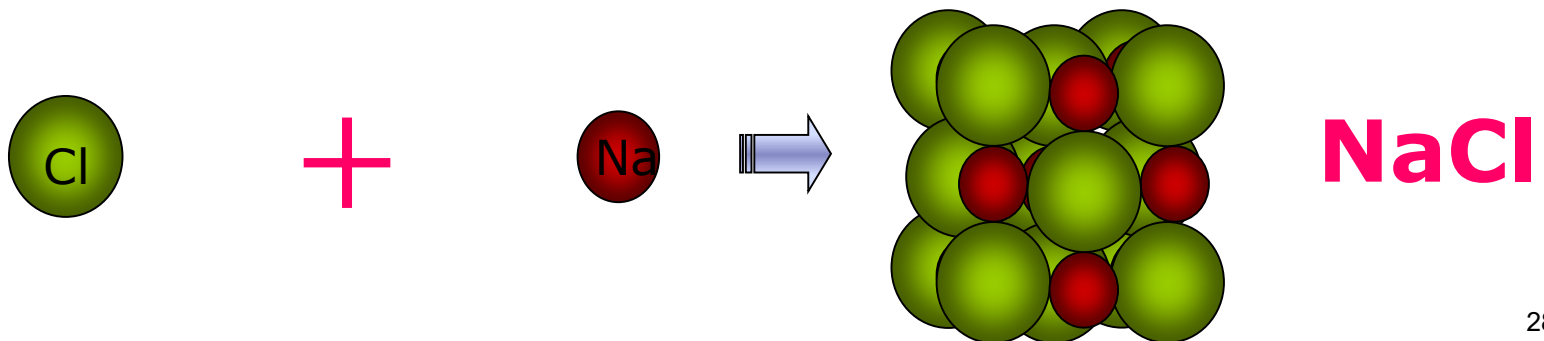
*What kind of forces hold the atoms together in a solid?*

- ❖ **Energies of Interactions Between Atoms**
- ❖ **Ionic bonding**
  - ✓ **NaCl**
- ❖ **Covalent bonding**
  - ✓ **Comparison of ionic and covalent bonding**
- ❖ **Metallic bonding**
- ❖ **Van der waals bonding**
- ❖ **Hydrogen bonding**



# Energies of Interactions between atoms

- The energy of the crystal is lower than that of the free atoms by an amount equal to the energy required to pull the crystal apart into a set of free atoms. This is called the binding (cohesive) energy of the crystal.
- NaCl is more stable than a collection of free Na and Cl.
- Ge crystal is more stable than a collection of free Ge.





# Types of Crystal Bonding

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It is conventional to classify the bonds between atoms into different types as

- ❑ Ionic
- ❑ Covalent
- ❑ Metallic
- ❑ Van der Waals
- ❑ Hydrogen

All bonding is a consequence of the electrostatic interaction between the nuclei and electrons.





# Ionic Bonding

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- Ionic bonding is the electrostatic force of attraction between positively and negatively charged ions (between non-metals and metals).
- All ionic compounds are crystalline solids at room temperature.
- NaCl is a typical example of ionic bonding.

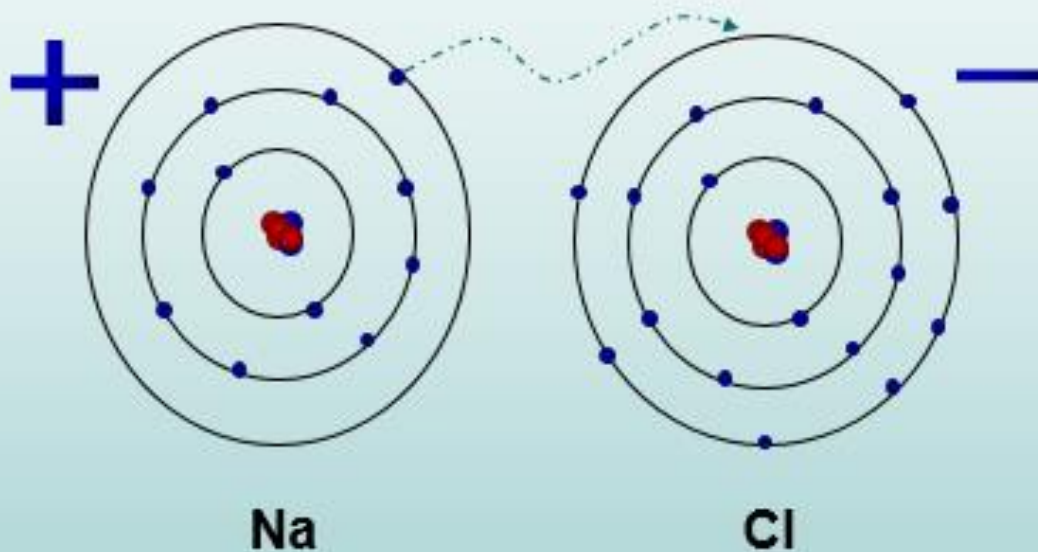


# Ionic Bonding

Metallic elements have only up to the valence electrons in their outer shell.

When losing their electrons they become positive ions.

Electronegative elements tend to acquire additional electrons to become negative ions or anions.





# Ionic Bonding

- When the  $\text{Na}^+$  and  $\text{Cl}^-$  ions approach each other closely enough so that the orbits of the electron in the ions begin to overlap with each other, then the electron begins to repel each other by virtue of the repulsive electrostatic coulomb force. Of course the closer together the ions are, the greater the **repulsive force**.



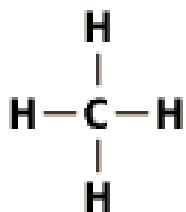
- Pauli exclusion principle has an important role in repulsive force. To prevent a violation of the exclusion principle, the potential energy of the system increases very rapidly.



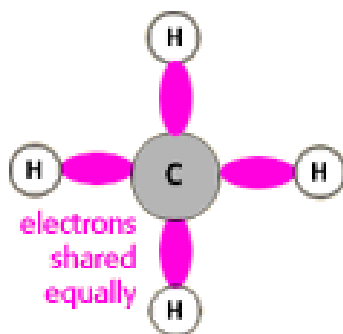
# Covalent Bonding

- Covalent bonding takes place between atoms with small differences in electronegativity which are close to each other in the periodic table (*between non-metals and non-metals*).
- The covalent bonding is formed when the atoms share the outer shell electrons (*i.e.*, *s* and *p* electrons) rather than by electron transfer.
- Noble gas electron configuration can be attained.

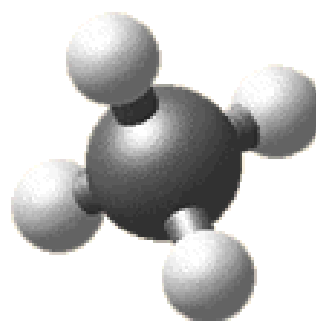
structural  
formula



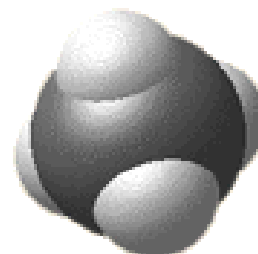
covalent  
bond diagram



ball & stick  
model



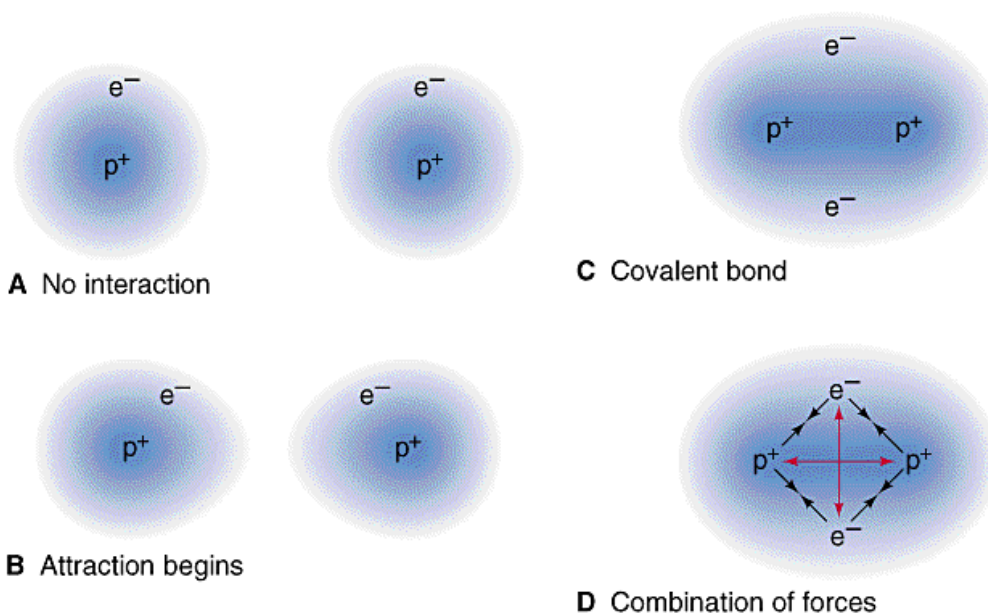
space-filling  
model





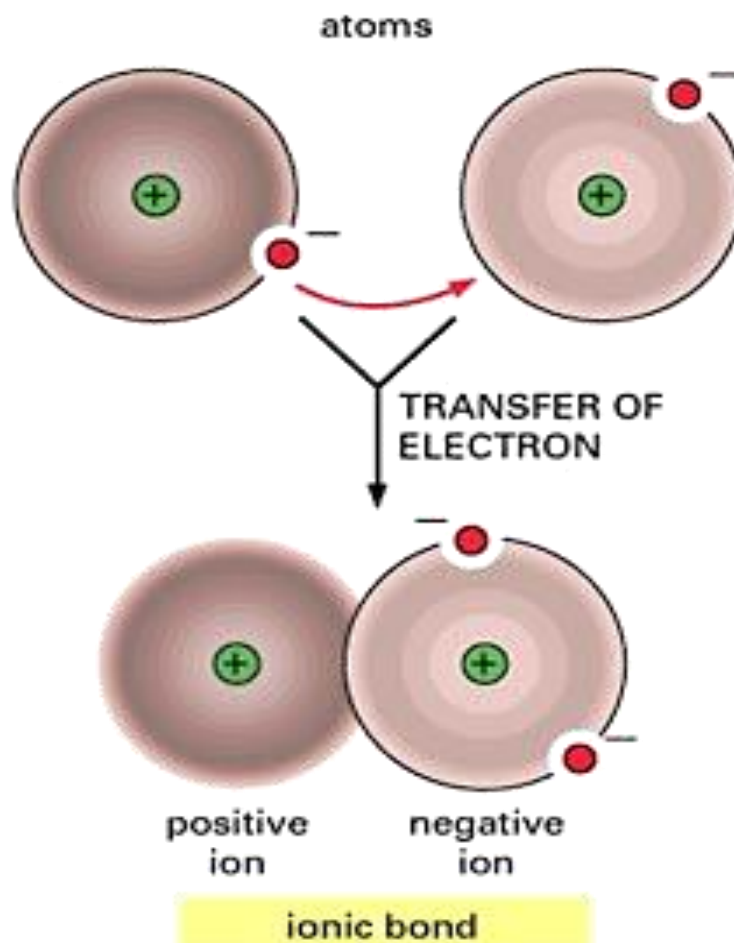
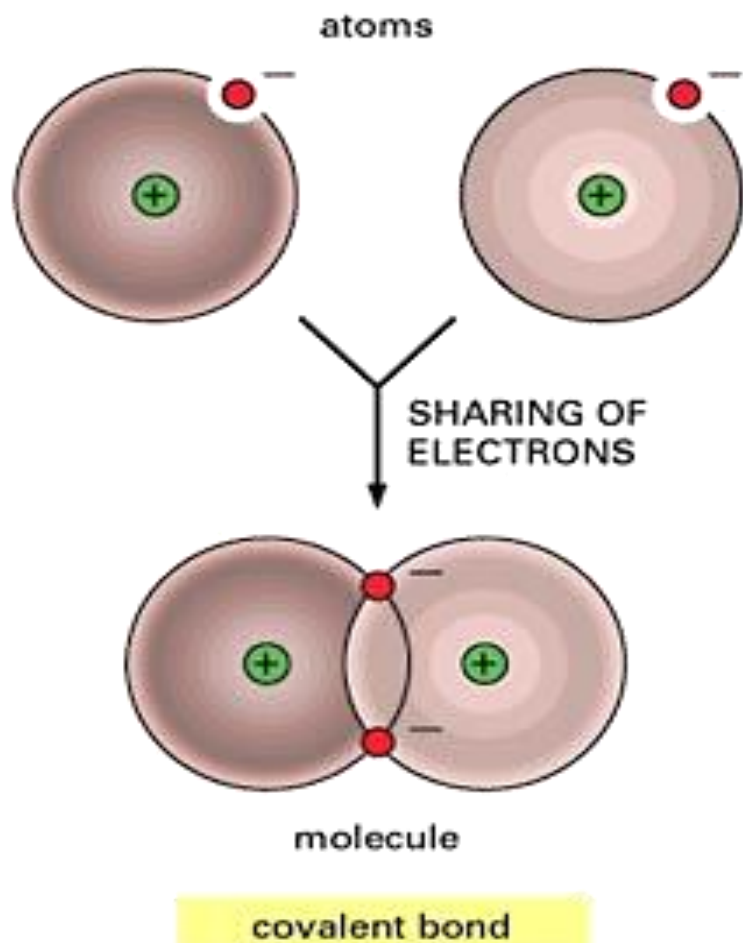
# Covalent Bonding

- Each electron in a shared pair is attracted to both nuclei involved in the bond. The approach, electron overlap, and attraction can be visualized as shown in the following figure representing the nuclei and electrons in a hydrogen molecule.





# Comparison of Ionic and Covalent Bonding

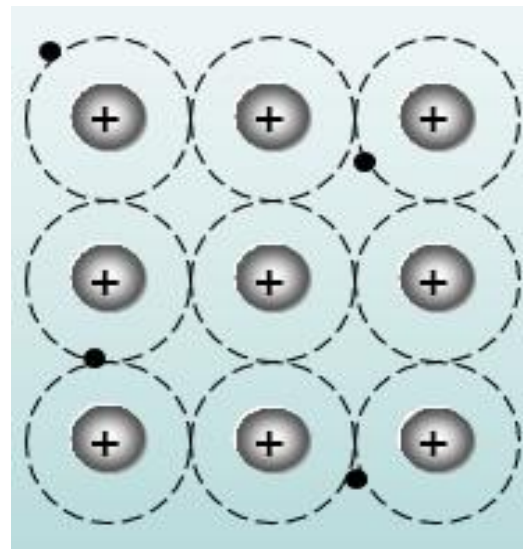
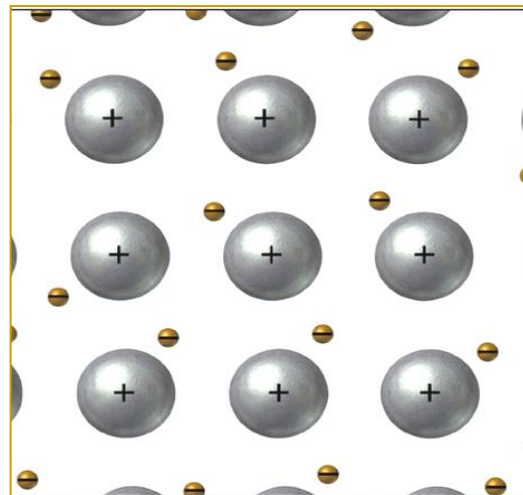






# Metallic Bonding

- ❑ Metallic bonding is found in metal elements. This is the electrostatic force of attraction between positively charged ions and delocalized outer electrons.
- ❑ The metallic bond is weaker than the ionic and the covalent bonds.
- ❑ A metal may be described as a low-density cloud of free electrons.
- ❑ Therefore, metals have high electrical and thermal conductivity.







# Van der Waal's Bonding

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- These are weak bonds with a typical strength of 0.2 eV/atom.
- Van Der Waals bonds occur between neutral atoms and molecules.
- Weak forces of attraction result from the natural fluctuations in the electron density of all molecules that cause small temporary dipoles to appear within the molecules.
- It is these temporary dipoles that attract one molecule to another. They are called van der Waals' forces.



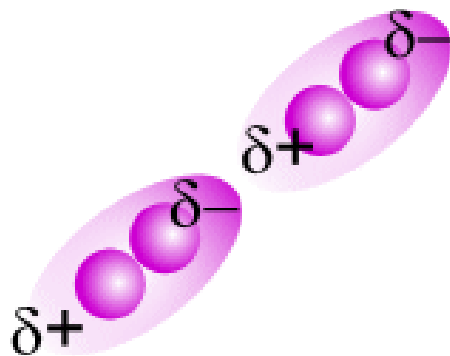
# Van der Waal's Bonding

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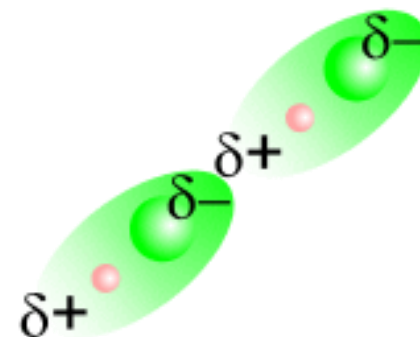
- The **shape** of a molecule influences its ability to form temporary dipoles. Long thin molecules can pack closer to each other than molecules that are more spherical. The bigger the 'surface area' of a molecule, the greater the van der Waal's forces will be and the higher the melting and boiling points of the compound will be.
- Van der Waal's forces are of the order of 1% of the strength of a covalent bond.



# Van der Waal's Bonding



Homonuclear molecules,  
such as iodine, develop  
temporary dipoles due to  
natural fluctuations of  
electron  
density within the molecule

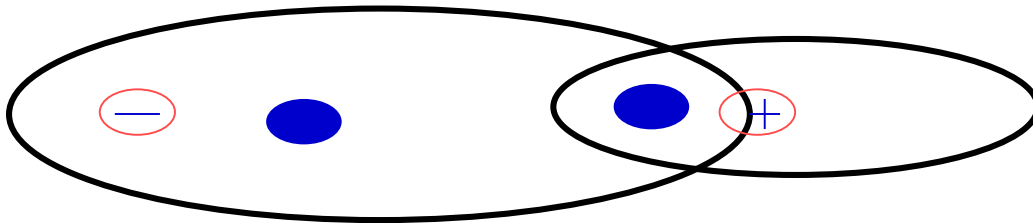


Heteronuclear molecules,  
such as H-Cl have permanent  
dipoles that attract the opposite  
pole in other molecules.

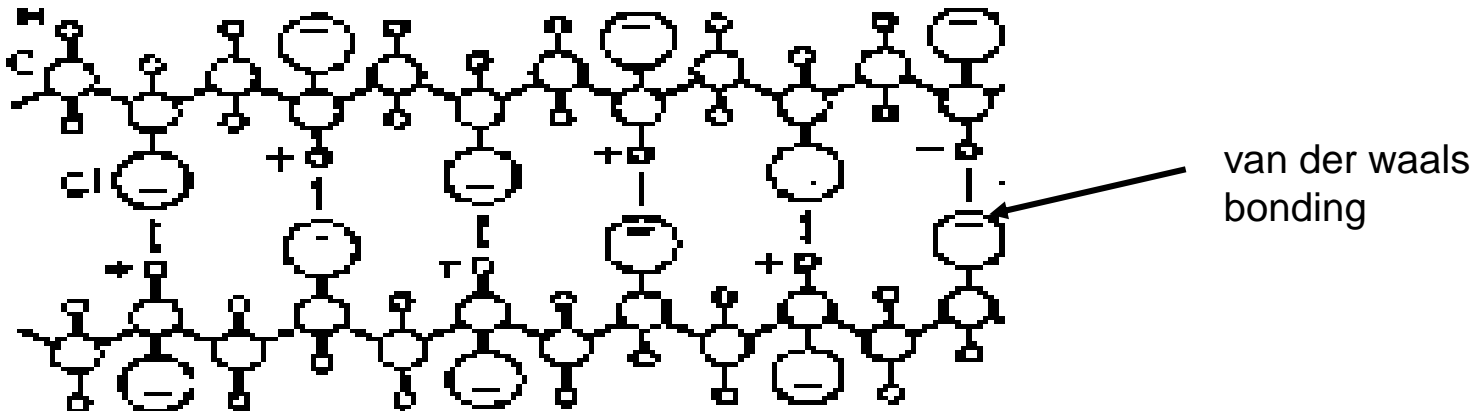


# Van der Waal's Bonding

- These forces are due to the electrostatic attraction between the nucleus of one atom and the electrons of the other.



- Van der waals interaction occurs generally between atoms which have noble gas configuration.





# Hydrogen Bonding

- A hydrogen atom, having one electron, can be covalently bonded to only one atom. However, the hydrogen atom can involve itself in an additional electrostatic bond with a second atom of highly electronegative character such as fluorine or oxygen. This second bond permits a **hydrogen bond** between two atoms or structures.
- The strength of hydrogen bonding varies from 0.1 to 0.5 eV/atom.
- Hydrogen bonds connect water molecules in ordinary ice. Hydrogen bonding is also very important in proteins and nucleic acids and therefore in life processes.



# Summary

## Types of Bonding

### Ionic Bonding

**High Melting Point**

**Hard and Brittle**

**Non conducting  
solid**

**NaCl, CsCl, ZnS**

### Van Der Waals Bonding

**Low Melting Points**

**Soft and Brittle**

**Non-Conducting**

**Ne, Ar, Kr and Xe**

### Metallic Bonding

**Variable Melting  
Point**

**Variable  
Hardness**

**Conducting**

**Fe, Cu, Ag**

### Covalent Bonding

**Very High Melting  
Point**

**Very Hard**

**Usually not  
Conducting**

**Diamond, Graphite**

### Hydrogen Bonding

**Low Melting Points**

**Soft and Brittle**

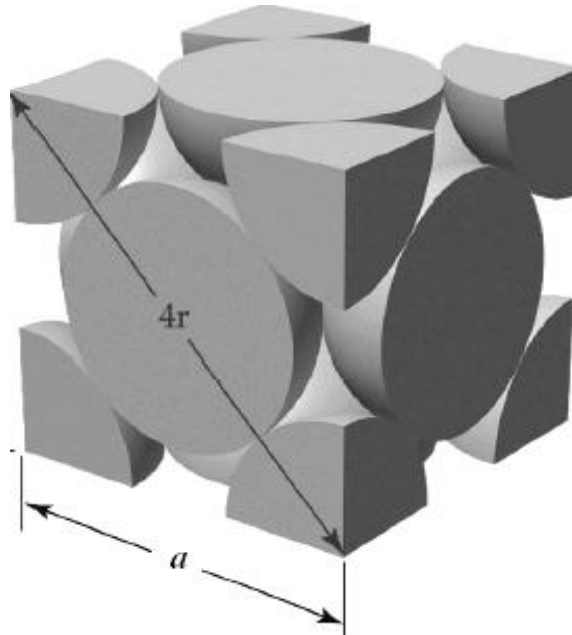
**Usually  
Non-Conducting**

**Ice,  
organic solids**



# Coordination Number

- Coordination number of a crystal is defined as the number of atoms or ions immediately surrounding a central atom in crystal system.



fcc structure



# Coordination Number

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- ✓ The atoms in an fcc unit cell touches along the face diagonal.
- ✓ Each and every corner atom is shared by eight adjacent unit cells.
- ✓ Therefore each and every corner atom contributes  $1/8$  of its part to one unit cell.
- ✓ So the total number of atoms contributed by the corner atoms is  $\left(\frac{1}{8}\right) \times 8 = 1$
- ✓ Two unit cells share each and every face centered atom.
- ✓ Therefore, the contribution of a face centered atom to unit cell is  $1/2$ .





# Coordination Number

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- ✓ So, the total number of atoms contributed by the face centered atoms =  $1/2 \times 6 = 3$ .
- ✓ The total number of atoms present in an fcc unit cell =  $1+3 = 4$ .



# Coordination Number of fcc Structure

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- ✓ In its own plane it touches four face centered atoms. The face centered atoms are its nearest neighbors.
- ✓ In a plane, which lies just above this corner atom, it has four more face centered atoms as nearest neighbors.
- ✓ Similarly, in a plane, which lies just below this corner atom it has yet four more face centered atoms as its nearest neighbors.
- ✓ Therefore the number of nearest neighbours *i.e.*, co-ordination number for fcc unit cell =  $4+4+4 = 12$



# Packing Fraction

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- Packing fraction is defined as the ratio of the total volume occupied by the set of objects/atoms packed into a space to the volume of the unit cell

Packing fraction i.e., the fraction of total volume filled:

$$PF = \frac{\text{Volume occupied by atoms}}{\text{Volume of the unit cell}}$$



# Home Work

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1. Show that the packing fraction of a face-centered cubic (fcc) structure is 0.74
2. Show that the packing fraction of a body-centered cubic (bcc) structure is 0.68
3. Prove that the direction  $[hkl]$  is the normal to the plane  $(hkl)$  for a cubic lattice.



# *Remember!!!*

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Packing fraction of an fcc is 0.74 means that 74 percent of the volume of the fcc unit cell is occupied by atoms and the remaining 26 percent volume of the unit cell is vacant or void space.



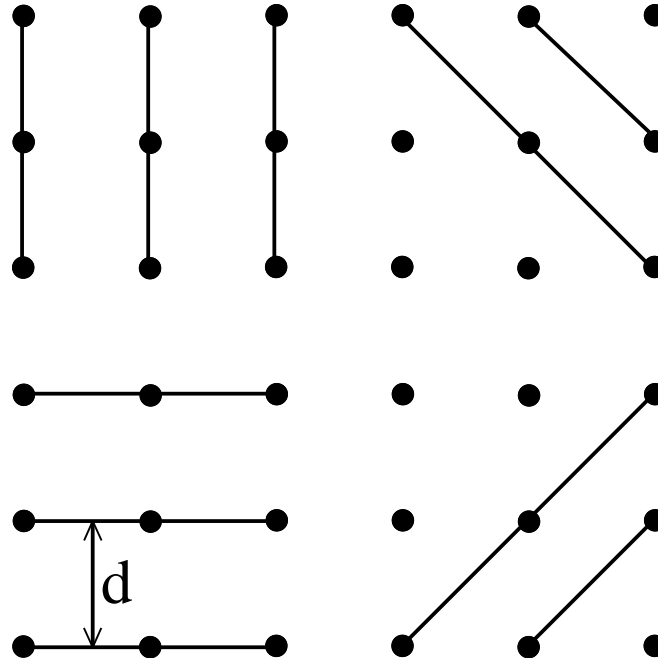
# Miller Indices

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- ✓ The crystal lattice may be regarded as made up of an infinite set of parallel equidistant planes passing through the lattice points which are known as lattice planes.
- ✓ In simple terms, the planes passing through lattice points are called '*lattice planes*'.
- ✓ For a given lattice, the lattice planes can be chosen in a different number of ways.



# Miller Indices



**Different Lattice Planes**



# Miller Indices

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- ✓ The orientation of planes or faces in a crystal can be described in terms of their intercepts on the three axes.
- ✓ Miller introduced a system to designate a plane in a crystal.
- ✓ He introduced a set of three numbers to specify a plane in a crystal.
- ✓ This set of three numbers is known as '*Miller Indices*' of the concerned plane.





# Miller Indices

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- ✓ Miller indices is defined as the reciprocals of the intercepts made by the plane on the three axes.



# Calculating Miller Indices

**Step 1:** Determine the intercepts of the plane along the axes  $X$ ,  $Y$ , and  $Z$  in terms of the lattice constants  $a$ ,  $b$  and  $c$ .

**Step 2:** Determine the reciprocals of these numbers.

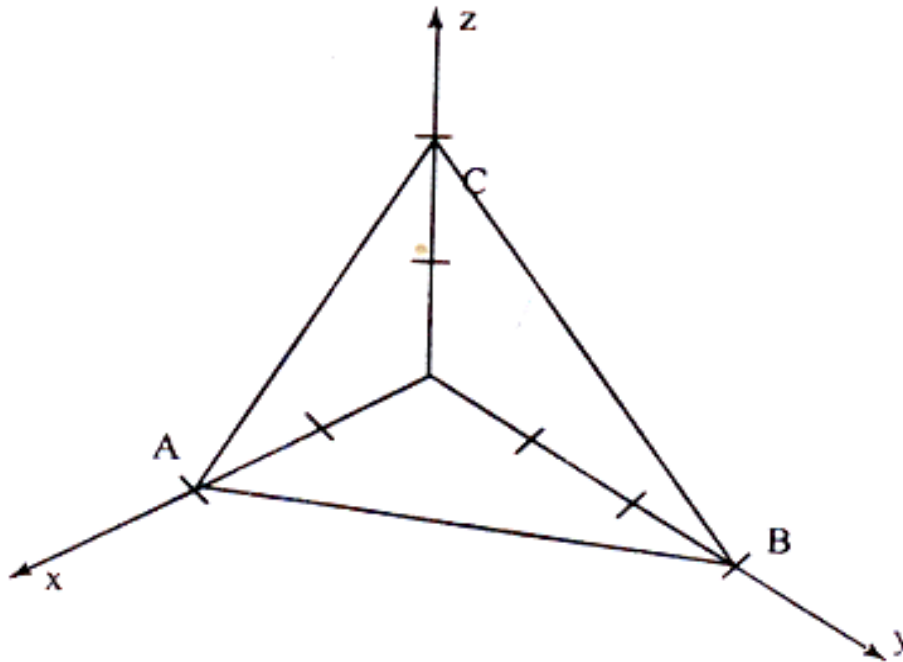
**Step 3:** Find the least common denominator ( $LCD$ ) and multiply each by this  $LCD$ .

**Step 4:** The result is written in parenthesis. This is called the ‘Miller Indices’ of the plane in the form  $(hkl)$ .

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## Determine the Miller Indices of the plane ABC



Plane ABC has intercepts of 2 units along X-axis, 3 units along Y-axis and 2 units along Z-axis.



## *Determine the Miller Indices of the plane ABC*

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**Step 1:** The intercepts are 2, 3, and 2 on the three axes.

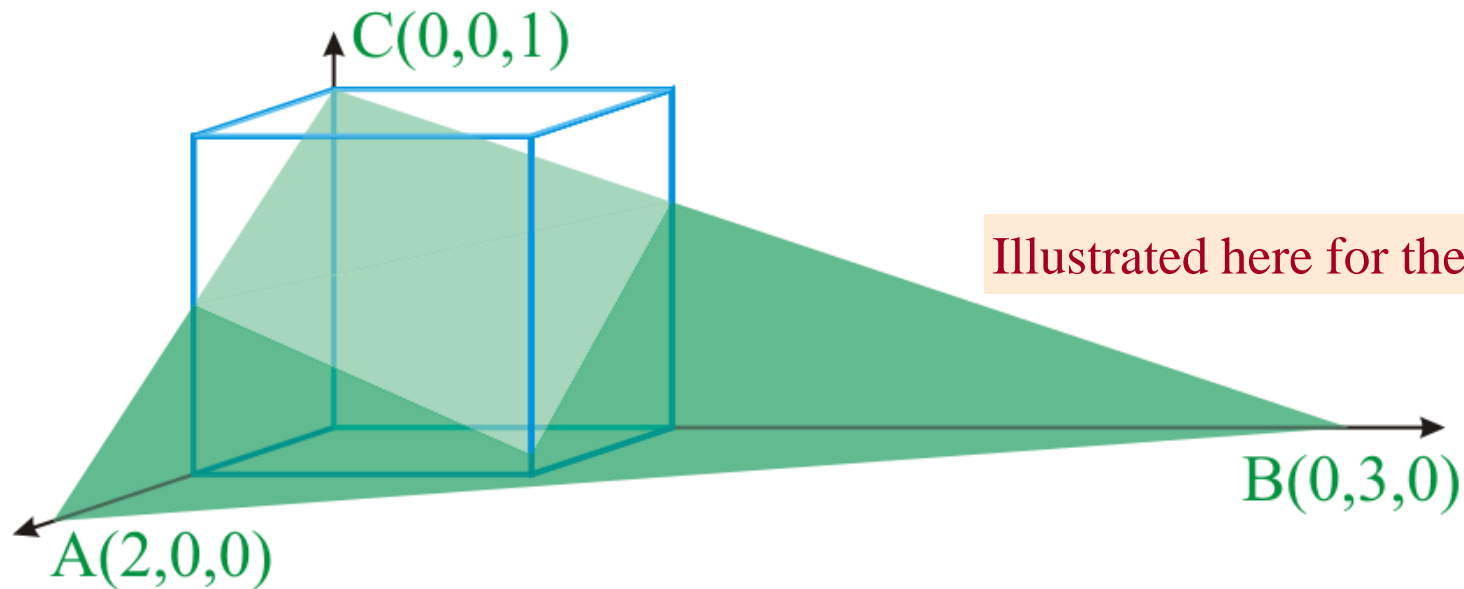
**Step 2:** The reciprocals are  $1/2$ ,  $1/3$  and  $1/2$ .

**Step 3:** The least common denominator is '6'. Multiplying each reciprocal by the 'LCD', we get 3, 2, and 3.

**Step 4:** Hence Miller indices for the plane ABC is (323)



# Determine the Miller Indices



Illustrated here for the cubic lattice

- ❑ Find intercepts along axes  $\rightarrow 231$
- ❑ Take reciprocals  $\rightarrow 1/2, 1/3, 1$
- ❑ Convert to smallest integers in the same ratio  $\rightarrow 326$
- ❑ Enclose in parenthesis  $\rightarrow (326)$



# Important Feature of Miller Indices

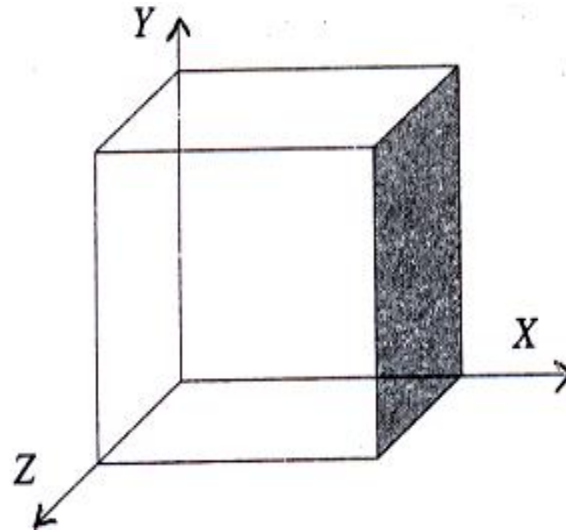
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- ✓ A plane which is parallel to any one of the co-ordinate axes has an intercept of infinity ( $\infty$ ). Therefore the Miller index for that axis is zero; *i.e.*, for an intercept at infinity, the corresponding index is zero.



# Example

**(100) plane**



**Plane parallel to Y and Z axes**



## Example

- ✓ In the above plane, the intercept along  $X$ -axis is 1 unit.
- ✓ The plane is parallel to  $Y$ -, and  $Z$ -axes. So, the intercepts along  $Y$ -, and  $Z$ -axes are ' $\infty$ '.
- ✓ Now the intercepts are 1,  $\infty$  and  $\infty$ .
- ✓ The reciprocals of the intercepts are  $= 1/1, 1/\infty$  and  $1/\infty$ .
- ✓ Therefore the Miller indices for the above plane is (100).



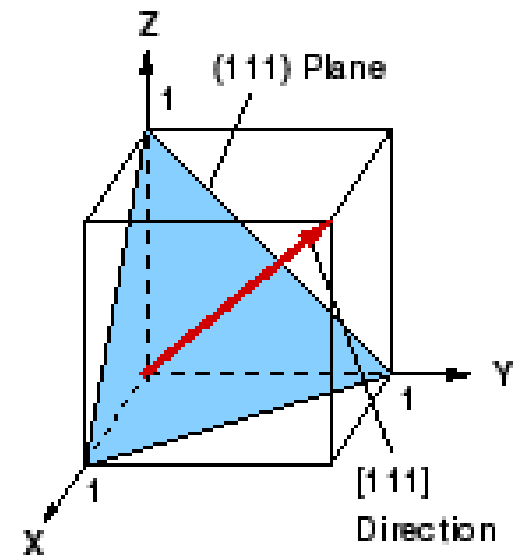
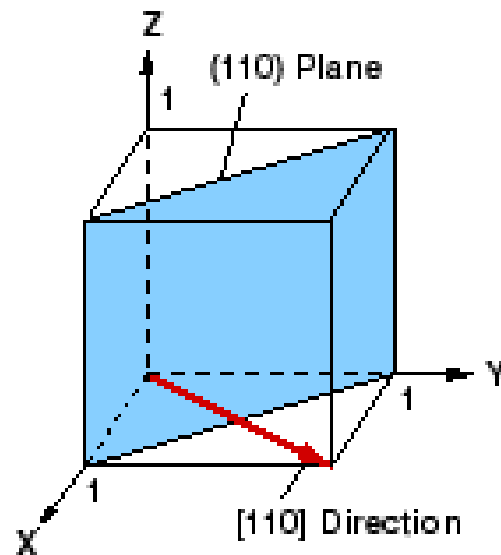
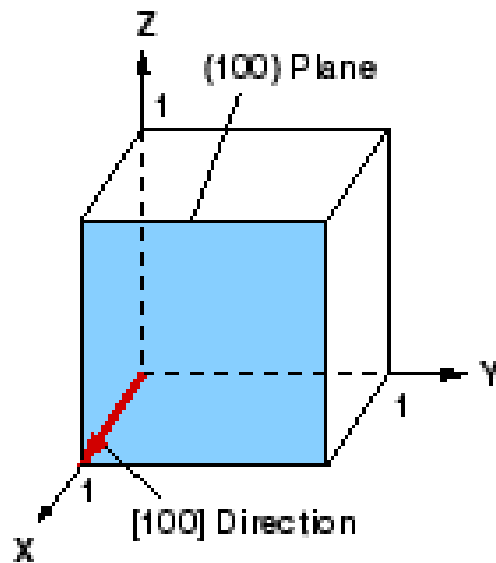


# Important Feature of Miller Indices

- ✓ A plane passing through the origin is defined in terms of a parallel plane having non zero intercepts.
- ✓ All equally spaced parallel planes have same 'Miller indices' *i.e.*, The Miller indices do not only define a particular plane but also a set of parallel planes. Thus the planes whose intercepts are 1, 1, 1; 2, 2, 2; -3, -3, -3 etc., are all represented by the same set of Miller indices.



# Structure of Matter





# Problems

1. A certain crystal has lattice parameters of 4.24, 10 and 3.66 Å on X, Y, Z axes respectively. Determine the Miller indices of a plane having intercepts of 2.12, 10 and 1.83 Å on the X, Y and Z axes.
2. Calculate the miller indices for the plane with intercepts  $2a$ ,  $-3b$ , and  $4c$  the along the crystallographic axes.
3. Find the angle between the directions  $[211]$  and  $[112]$  in a cubic crystal.



# Plane and Direction Relations

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Planes and directions that share the indices are perpendicular

$[hkl]$  is perpendicular to  $(hkl)$

$$\cos(\theta) = \frac{(hu + kv + lw)}{(h^2 + k^2 + l^2)^{1/2} \cdot (u^2 + v^2 + w^2)^{1/2}}$$



# Answers to the Problems

## Solution to Problem # 1

Lattice parameters are = 4.24, 10 and 3.66 Å

The intercepts of the given plane = 2.12, 10 and 1.83 Å

i.e. The intercepts are, 0.5, 1 and 0.5.

Step 1: The Intercepts are  $1/2$ , 1 and  $1/2$ .

Step 2: The reciprocals are 2, 1 and 2.

Step 3: The least common denominator is 2.

Step 4: Multiplying the LCD by each reciprocal we get, 4, 2 and 4.

Step 5: By writing them in parenthesis we get (424)

**Therefore the Miller indices of the given plane is (424) or (212).**





# Answers to the Problems

## Solution to Problem # 2

The intercepts are 2, -3 and 4

Step 1: The intercepts are 2, -3 and 4 along the 3 axes

Step 2: The reciprocals are  $\frac{1}{2}$ ,  $\frac{1}{-3}$  and  $\frac{1}{4}$

Step 3: The least common denominator is 12.

Multiplying each reciprocal by lcd, we get 6 -4 and 3

Step 4: Hence the Miller indices for the plane is  $(6 \bar{4} 3)$



# Answers to the Problems

## Solution to Problem # 3

The two directions are  $[2 \ 1 \ 1]$  and  $[1 \ 1 \ 2]$

We know that the angle between the two directions,

$$\cos \theta = \frac{u_1 u_2 + v_1 v_2 + w_1 w_2}{(u_1^2 + v_1^2 + w_1^2)^{1/2} \times (u_2^2 + v_2^2 + w_2^2)^{1/2}}$$

In this case,  $u_1 = 2, v_1 = 1, w_1 = 1, u_2 = 1, v_2 = 1, w_2 = 2$

$$\therefore \cos \theta = \frac{(2 \times 1) + (1 \times 1) + (1 \times 2)}{\sqrt{2^2 + 1^2 + 1^2} \times \sqrt{1^2 + 1^2 + 2^2}} = \frac{5}{6}$$

Or,  $\cos \theta = 0.833$

$\theta = 35^\circ 35'30''$ .



# Relationship between $d$ , Miller indices

The relationship between  $d$ , Miller indices and the lattice parameters

Crystal system	$d_{hkl}$ , lattice parameters and Miller indices
Cubic	$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$
Tetragonal	$\frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$
Orthorhombic	$\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$

The expressions for the remaining crystal systems are more complex





# Relationship between $d$ , Miller indices

The relationship between  $d$ , Miller indices and the lattice parameters

Monoclinic

$$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2 \sin^2 \gamma} + \frac{k^2}{b^2 \sin^2 \gamma} - \frac{2hk \cos \gamma}{ab \sin^2 \gamma} + \frac{l^2}{c^2}$$

Hexagonal

$$\frac{1}{d_{hkl}^2} = \left[ \frac{4}{3} (h^2 + k^2 + hk) + l^2 \left( \frac{a}{c} \right)^2 \right] \frac{1}{a^2}$$

The expressions for the remaining crystal systems are even more complex



Thank You for Listening

Physics is hopefully simple but Physicists are not

