SOLIDS

CLASSIFICATIONS OF SOLIDS

There are two main categories of solids: Crystalline and amorphous.

Crystalline solids

- *have atoms arranged in an orderly repeating pattern*
- *are well ordered at the atomic level*
- *have a specific geometric shape*
- *have a constant melting point*

Ex: glass, rubber, plastic

Amorphous solids

- *lack the order found in crystalline solids*
- *are disordered*
- *do not have a specific geometric shape*
- *do not have a certain melting point, become fluent in a certain temperature range called as the glass transition temperature* (T_g)

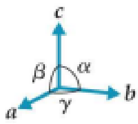
Ex: NaCl, Cu, Ar

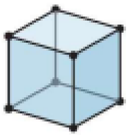
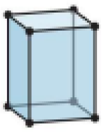
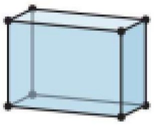
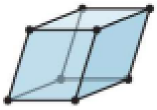
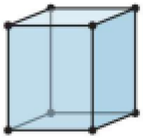
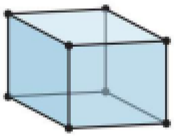
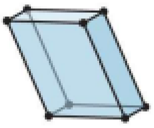
CLASSIFICATIONS OF CRYSTALS

1. *According to the unit cell type*
2. *According to the structural units in the lattice points*
3. *According to the occupying of atoms into the cavities*

CRYSTAL TYPES DEPENDING ON THE UNIT CELL TYPE

The unit cell is a relatively small repeating unit that is made up of a unique arrangement of atoms and embodies the structure of the solid.

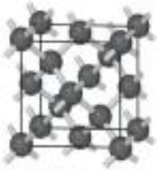
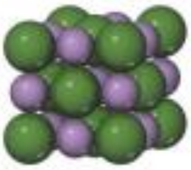


	*CUBIC*	$a=b=c$	$\alpha=\beta=\gamma=90^o$	*Primitive* *Body-centered* *Face-centered*
	*TETRAGONAL*	$a=b\neq c$	$\alpha=\beta=\gamma=90^o$	*Primitive* *Body-centered*
	*ORTHORHOMBIC*	$a\neq b\neq c$	$\alpha=\beta=\gamma=90^o$	*Primitive* *Body-centered* *Face-centered* *Base-centered*
	*RHOMBOHEDRAL*	$a=b=c$	$\alpha=\beta=\gamma\neq 90^o<120^o$	
	*HEXAGONAL*	$a=b\neq c$	$\alpha=\beta=90^o$, $\gamma=120^o$	
	*MONOCLINIC*	$a\neq b\neq c$	$\alpha=\beta=90^o$, $\gamma\neq 120^o$	*Primitive* *Base-centered*
	*TRICLINIC*	$a\neq b\neq c$	$\alpha\neq\beta\neq\gamma\neq 90^o$	

CRYSTAL TYPES DEPENDING ON THE STRUCTURAL UNITS IN THE LATTICE POINTS

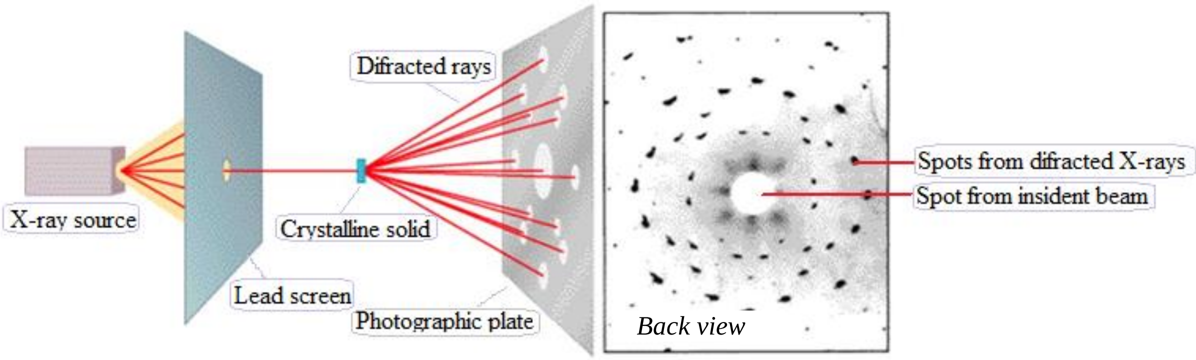
There are four different types of crystalline solids:

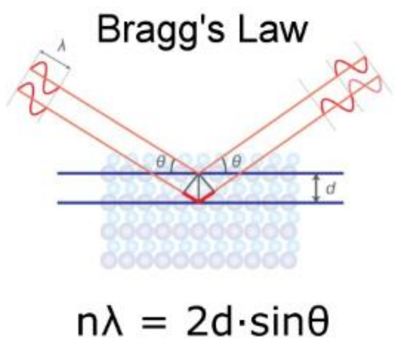
1. *Metallic solids*
2. *Ionic solids*
3. *Covalent solids*
4. *Molecular solids*

		Structural Unit in the Lattice Point	*Properties*	*Examples*
	*Covalent solids*	*Covalently bonded atom*	*Hard, high melting and boiling points*	*Diamond, graphite*
	*Ionic solids*	*(+) and (-) charged ions [electrostatic force (pull force)]*	*Hard, high melting and boiling points*	*NaCl, KBr, LiF*
	*Metallic solids*	*Metal cations in the electron cloud [electrostatic force]*	*Variable hardness, melting and boiling points, conductive*	*Au, Ag, Cu, Fe*
	*Molecular solids*	*Molecules (dipol-dipol and Van der Waals interactions)*	*Soft, low melting and boiling points, nonconductive*	*H_2O, naphthalene, sulfur, sugar*

CLARIFICATIONS OF CRYSTAL STRUCTURES USING X-RAY CRYSTALLOGRAPHY

X-ray crystallography is the technique used to determine the crystal structure of crystalline solids (known or unknown) based on their diffraction pattern.





IN BRAGG EQUATION

n *is an integer*

the variable ***λ*** *is the characteristic the wavelength of the incident X-rays impinging on the crystallize sample*

the variable ***d*** *is the distance between atomic layers in a crystal*

θ *is the angle of the X-ray beam with respect to these planes*

IONIC SOLIDS

Radius Ratio (r^+/r^-)

The radius ratio can be calculated if ionic radii are known, coordination number and geometric structure can be defined.

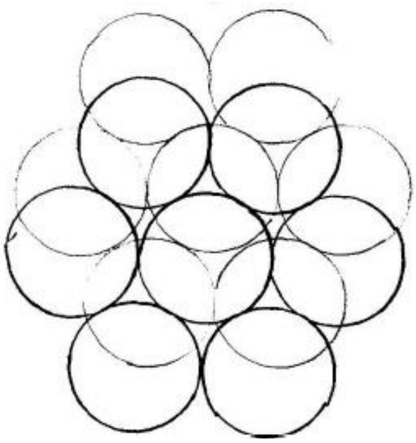
Radius ratio (r^+/r^-)	**Coordination number**	**Geometry**
< 0.155	2	Linear
0.155-0.225	3	Trigonal planar
0.225-0.414	4	Tetrahedron
0.414-0.732	4	Square planar
0.414-0.732	6	Octahedron
0.732-0.999	8	Body-centered cubic

Crystal Faults

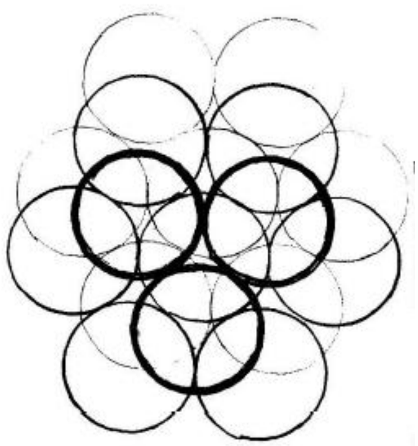
In many crystals, some unit cells are empty or some unit cells are shifted.

Close Packing

The gap ratio is possible in two different ways, provided that it remains the same: 1) Cubic close packing. 2) Hexagonal close packing.



Hexagonal close packing



Cubic close packing

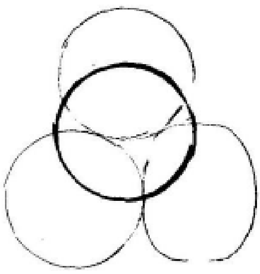
Close packing also includes 3 types of cavities:

1. *Tetrahedral cavities*
2. *Octahedral cavities*
3. *Cubic cavities*

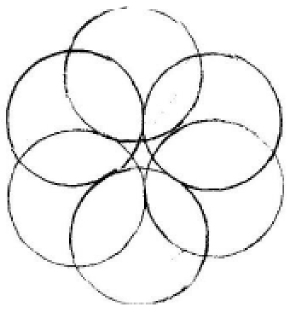
Tetrahedral cavities: The cavity formed by the contact of four spheres.

Octahedral cavities: The cavity formed by six spheres.

Cubic cavities: In most ionic crystals, the larger ion (usually anion) forms one of the primitive, body-centered or face-centered cubic lattices as sub-lattices. Cations fill the cavities of these lattices.



Tetrahedral cavity



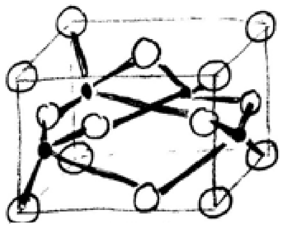
Octahedral cavity

Formula	*Example*	*Type of close packing*	*The occupancy of cavities*		*Coordination*
			Tetrahedral	***Octahedral***	***number***
AX	*NaCl*	*ccp*	-		*6:6*
	NiAs	*hcp*	-		*6:6*
	ZnS (zinc blende)	*ccp*	$^1/_2$	-	*4:4*
	ZnS (wurtzite)	*hcp*	$^1/_2$	-	*4:4*
AX_2	*CaF_2*	*ccp*		-	*4:8*
	CdI_2	*hcp*	-	$^1/_2$	*6:3*
	$CdCl_2$	*ccp*	-	$^1/_2$	*6:3*
	β-$ZnCl_2$	*hcp*	$^1/_4$	-	*4:2*
	HgI_2	*ccp*	$^1/_4$	-	*4:2*
AX_3	*BiI_3*	*hcp*	-	$^1/_3$	*6:2*
	$CrCl_3$	*ccp*	-	$^1/_3$	*6:2*
AX_4	*SnI_4*	*hcp*	$^1/_8$	-	*4:1*
AX_6	*α-WCl_6, UCl_6*	*ccp*	$^1/_8$	$^1/_6$	*6:1*
A_2X_3	*Al_2O_3 (corundum)*	*hcp*		$^2/_3$	*6:4*

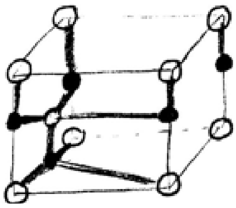
CRYSTAL TYPES DEPENDING ON THE CHOICE OF ATOMS TO FILL IN CAVITIES (CLASSIFICATION OF IONIC STRUCTURES)

AX TYPE COMPOUNDS

a. Zinc sulfide structure

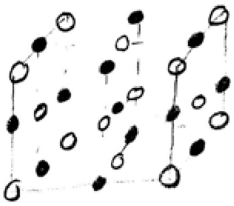


Zinc blende

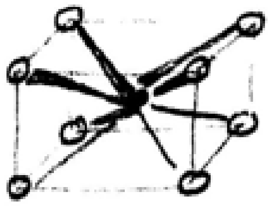


Wurtzite

b. Sodium chloride structure (rock salt, halite)



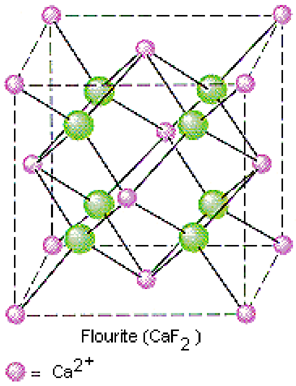
c. Cesium chloride structure



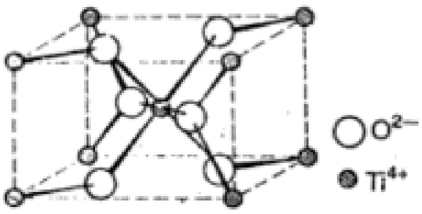
	CsCl	NaCl	ZnS
r^+ (Å)	1.81	1.16	0.88
r^- (Å)	1.67	1.67	1.70
r^+/r^-	1.08	0.69	0.52
Coordination number of cation	8	6	4
Coordination number of anion	8	6	4

AX_2 TYPE COMPOUNDS

a. Calcium Floride (Fluorite) Structure



b. Rutile Structure



c. β-cristobalite (silica) structure

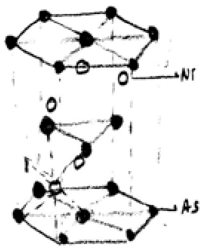
Silica (SiO_2) has six crystal structures called quartz, cristobalite and tridimide, each of which has an α and β form. The radius ratio indicates the coordination number is 4 and the cytokiometry is 4:2.

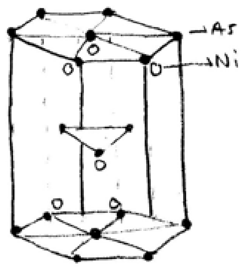
LAYERED STRUCTURES

a. Cadmium iodide structure

b. Cadmium chloride structure

c. Nickel arsenide structure





STRUCTURES CONTAINING POLYATOMIC IONS

OTHER LATTICES

CRYSTAL LATTICE DEFECTS

1. *Lattice blanks*
2. *Lattice cracks*
3. *f-Centered crystals*
4. *Crystal impurities*

FACTORS DETERMINING THE TYPE OF LATTICE

1. *Stoichiometry*
2. *Radius ratio*
3. *Covalent character*