

# ELE 362: Structures of Materials

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# SOLIDS

## CRYSTALLINE

**$10^{28}$  atoms/m<sup>3</sup>**

**Regular arrangement  
Basic building blocks are  
unit cells**

**Portions perfect--  
polycrystalline--  
grain boundaries**

## AMORPHOUS

**Crystallites approach size  
of unit cell, i.e. A ( $10^{-10}$  m)**

**NO LONG RANGE ORDER**

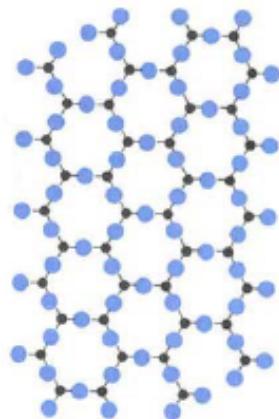
**Crystalline** solids have of the order of  $10^{28}$  atoms/cubic meter and have a regular arrangement of atoms.

**Amorphous** solids have about the same density of atoms, but lack the long range order of the crystalline solid (usually no greater than a few Angstroms). Their crystallites approach the order of the unit cell. The basic building blocks of crystalline materials are the unit cells which are repeated in space to form the crystal. However, most of the materials which we encounter (eg. a copper wire, a horseshoe magnet, a sugar cube, a galvanized steel sheet) are what we call **polycrystalline**. This word implies that portions of the solid are perfect crystals, but not all of these crystals have the same axis of symmetry. Each of the crystals (or grains) have slightly different orientations with boundaries bordering on each other. These borders are called **grain boundaries**.

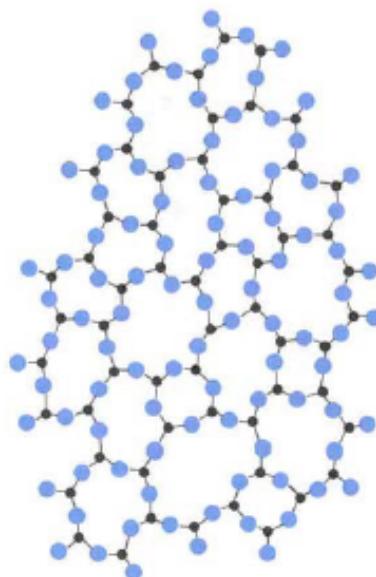
# Crystalline and amorphous solids

A crystalline material is one in which the atoms are situated in a repeating or periodic array over large atomic distances.

Long-range order occurs upon solidification from the liquid state.



Crystal



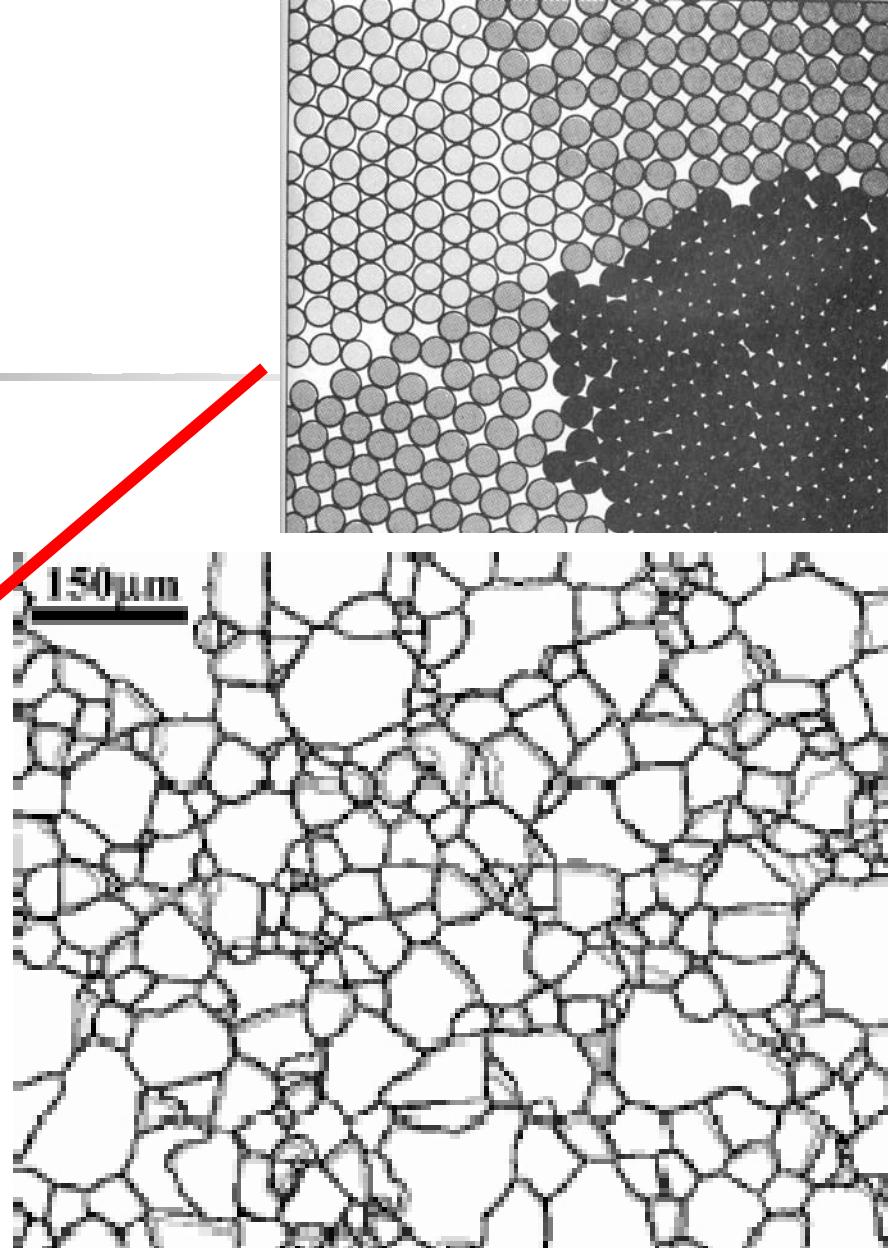
Amorphous solid

For materials that do not crystallize, no long-range order occurs and these materials are noncrystalline, or amorphous.

# Polycrystals and grain boundaries

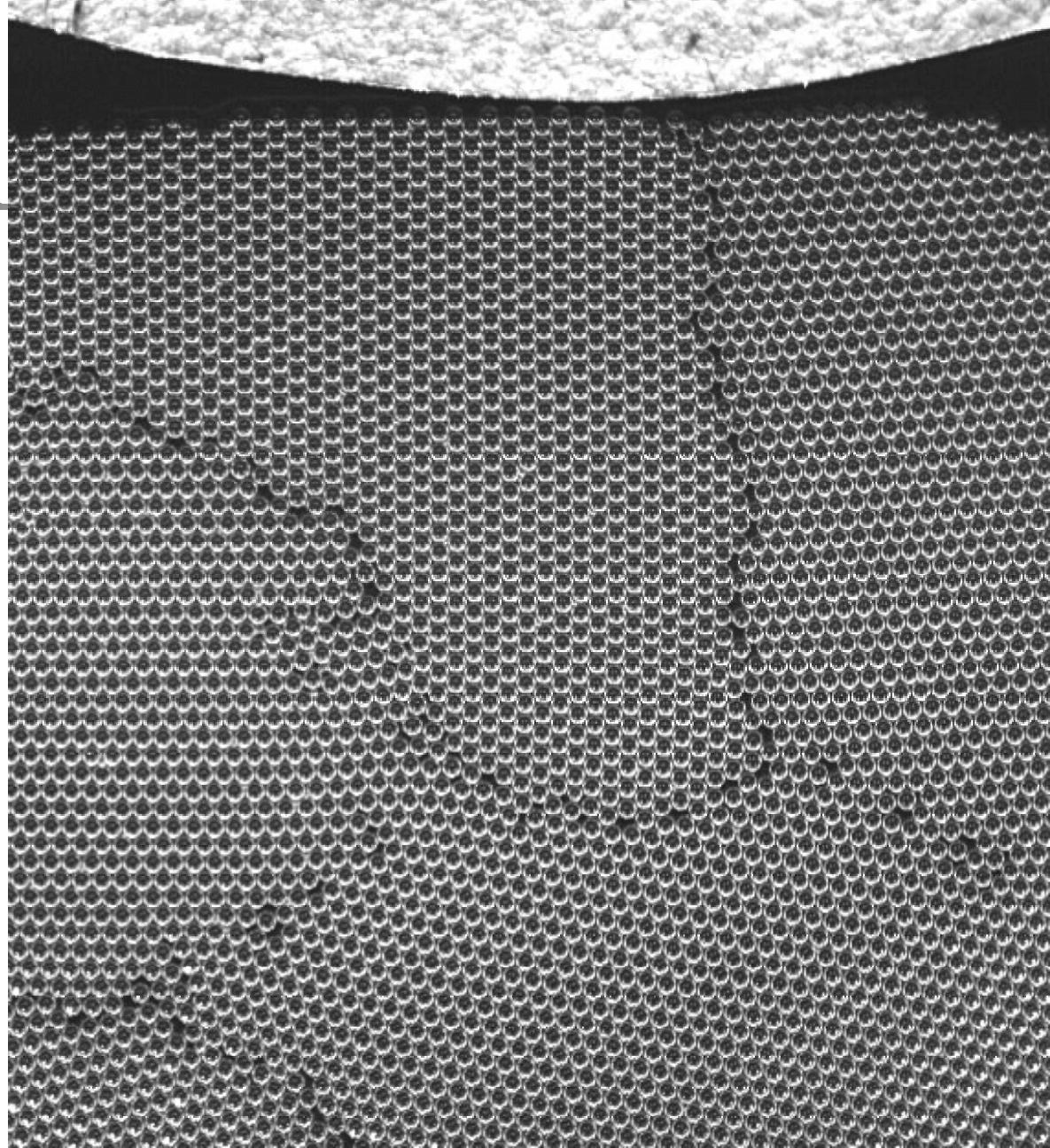
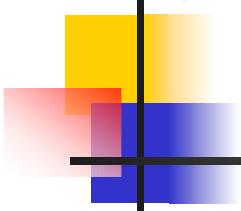


Quartz



A superposition of the grain boundary traces from adjacent layers in the microstructure of MgO. The vertical separation is about 5  $\mu\text{m}$  [4].

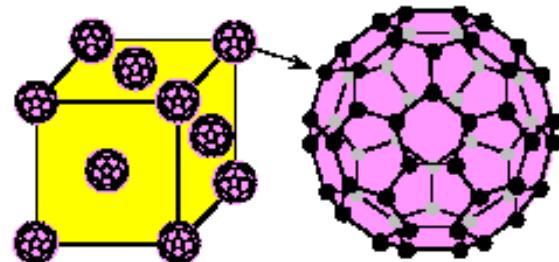
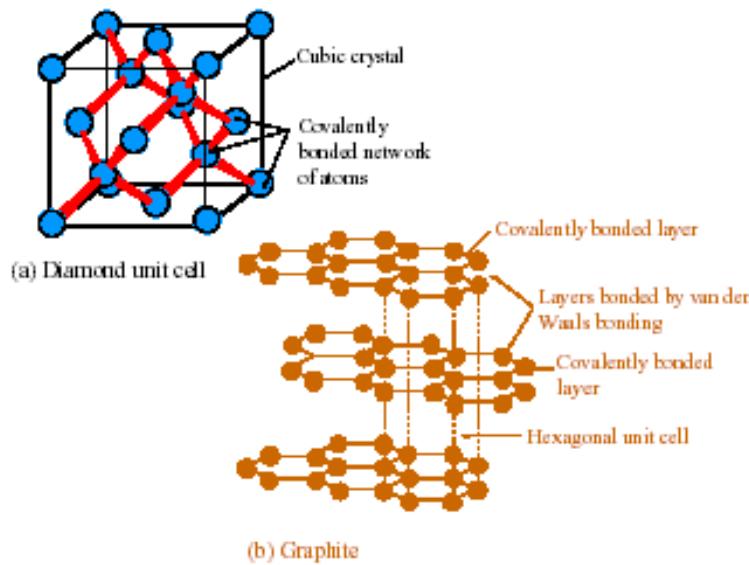
# Polycrystal G.B. Movement



# Crystalline allotropes of carbon ( $\rho$ is the density and $Y$ is the elastic modulus or Young's modulus)

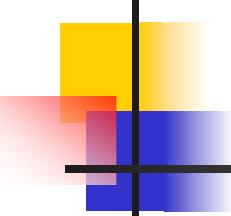
	Graphite	Diamond	Buckminsterfullerene Crystal
<b>Structure</b>	Covalent bonding within layers. Van der Waals bonding between layers. Hexagonal unit cell.	Covalently bonded network. Diamond crystal structure.	Covalently bonded $C_{60}$ spheroidal molecules held in an FCC crystal structure by van der Waals bonding.
<b>Electrical And Thermal Properties</b>	Good electrical conductor. Thermal conductivity comparable to metals.	Very good electrical insulator. Excellent thermal conductor, about 5 times more than silver or copper.	Semiconductor. Compounds with alkali metals (e.g. $K_3C_{60}$ ) exhibit superconductivity.
<b>Mechanical Properties</b>	Lubricating agent. Machinable. Bulk graphite: $Y \approx 27 \text{ GPa}$ , $\rho = 2.25 \text{ g cm}^{-3}$	The hardest material. $Y = 827 \text{ GPa}$ $\rho = 3.5 \text{ g cm}^{-3}$	Mechanically soft. $Y \approx 18 \text{ GPa}$ $\rho = 1.65 \text{ g cm}^{-3}$
<b>Comment</b>	Stable allotrope at atmospheric pressure.	High pressure allotrope.	Laboratory synthesized. Occurs in the soot of partial combustion.
<b>Uses, Potential Uses</b>	Metallurgical crucibles, welding electrodes heating elements, electrical contacts, refractory applications.	Cutting tool applications. Diamond anvils. Diamond film coated drills, blades, bearings etc. Jewelry. Heat conductor for ICs. Possible thin film semiconductor devices as the charge carrier drift mobilities are large.	Possible future semiconductor or superconductivity applications.

# Pictorial of carbon allotropes



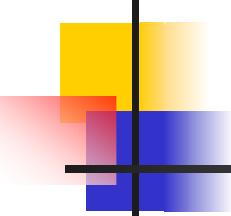
(c) Buckminsterfullerene

NOTE: there is also a Quasi-allotrope called **Diamond-like carbon**



# Crystalline and amorphous silicon

	Crystalline Si c-Si	Amorphous Si a-Si	Hydrogenated a-Si a-Si:H
<b>Structure</b>	Diamond cubic.	Short range order only. On average, each Si covalently bonds with four Si atoms. Has microvoids and dangling bonds	Short range order only. Structure contains typically 10% H. Hydrogen atoms passivate dangling bonds and relieve strain from bonds.
<b>Typical Preparation</b>	Czochralski technique	Electron beam evaporation of Si	Chemical vapor deposition (CVD) of silane gas by RF (radio frequency) plasma.
<b>Density g cm<sup>-3</sup></b>	2.33	About 3-10% less dense.	About 1-3% less dense
<b>Electronic Applications</b>	Discrete and integrated electronic devices.	None	Large area electronic devices such as solar cells, thin film transistor arrays in flat panel displays and photoconductor drums used in photocopying.



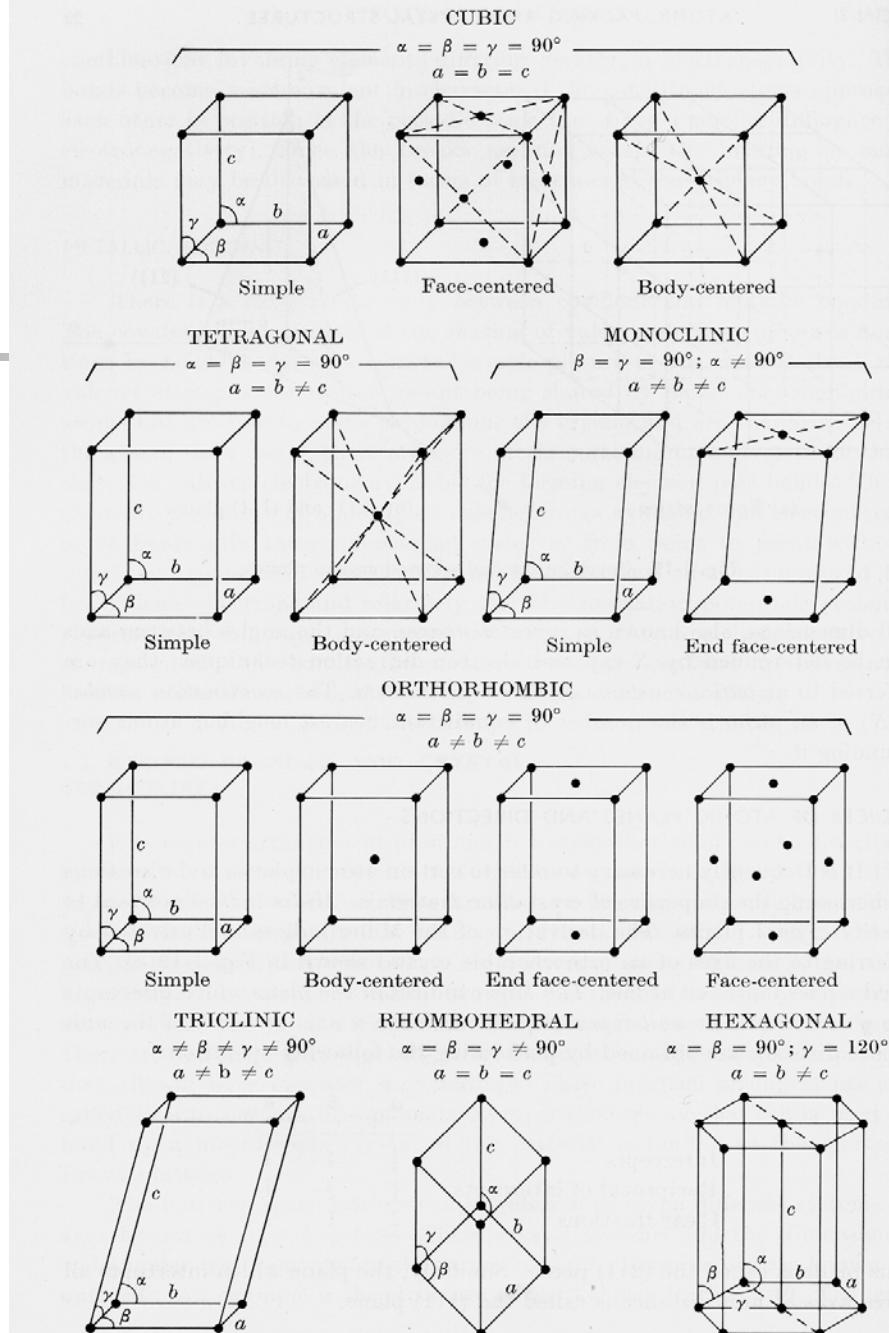
# Crystal Systems

name	dimensions	angles
isometric (cubic)	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$
tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$
orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$
monoclinic	"	$\alpha = \gamma = 90^\circ \neq \beta$
triclinic	"	$\alpha, \beta, \gamma \neq 90^\circ$
trigonal*	"	
hexagonal	$a_1 = a_2 = a_3 \neq c$	$a_i \wedge a_j = 120^\circ, a_i \wedge c = 90^\circ$

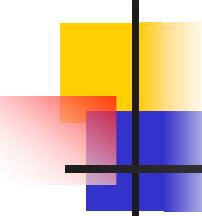
\*used only in Europe. In America, trigonal is a special case of hexagonal.

# Bravais Lattices

- In 1850, Auguste Bravais showed that crystals could be divided into 14 unit cells, which meet the following criteria.
  - The unit cell is the simplest repeating unit in the crystal.
  - Opposite faces of a unit cell are parallel.
  - The edge of the unit cell connects equivalent points.
- The 14 Bravais unit cells are shown in the figure adjacent

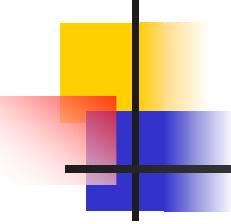


The fourteen Bravais lattices and the seven crystal systems.<sup>1</sup>



# THE UNIT CELL

- In order to further our knowledge and ability to apply the principals of atomic and crystalline structure to the problems at hand, we must first define a concept on which hinges the rest of crystallography. This concept is the unit cell.
- The unit cell is defined as the smallest group of atoms which, by repeated translation in three dimensions, builds up the whole crystal. This means that the unit cell consists only of those atoms which exclusively belong to that basic building block.
- The concept is better shown in pictorial fashion for three of the cubic crystal types



# Number of Atoms per Unit Cell

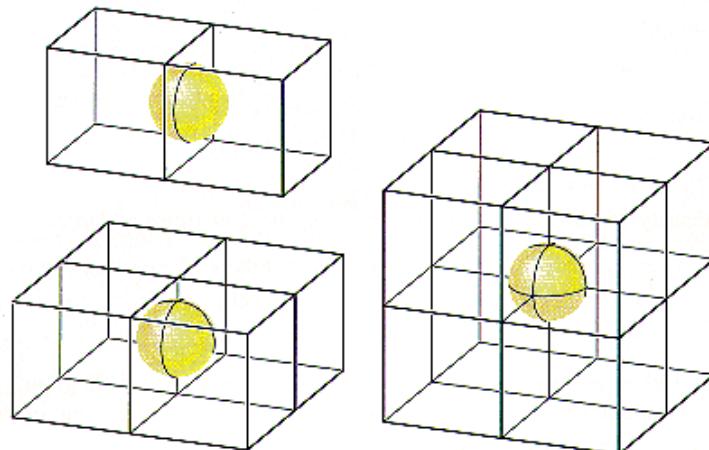
In a mathematical way, for the cubic lattice, the number of atoms per unit cell is given by

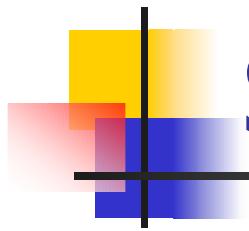
$$N = N(c)/8 + N(i) + N(f)/2$$

where  $N$  is the number of atoms per unit cell,  $N(c)$  is the number of corner atoms (shared by eight),  $N(i)$  is the number of internal atoms (shared by none), and  $N(f)$  is the number of face atoms (shared by two). So, for the BCC and FCC, the number of atoms per unit cell are 2 and 4 respectively. Similar calculations can be performed for other lattices.

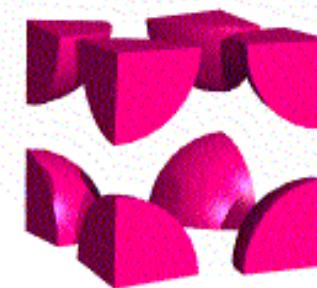
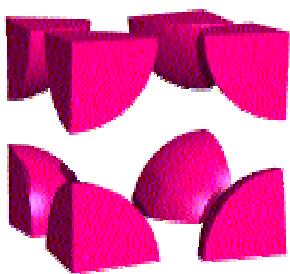
# *Determining the Unit Cell of a Crystal*

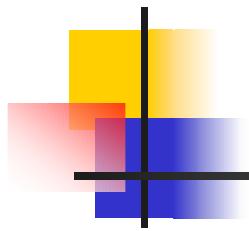
- Atoms on the corners, edges, and faces of a unit cell (cubic) are shared by more than one unit cell, as shown in the figure below.
- An atom on a face is shared by two unit cells, so only half of the atom belongs to each of these cells.
- An atom on an edge is shared by four unit cells, and an atom on a corner is shared by eight unit cells.
- Thus, only one-quarter of an atom on an edge and one-eighth of an atom on a corner can be assigned to each of the unit cells that share these atoms.



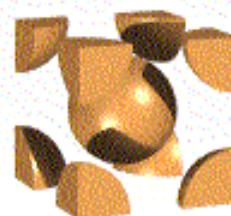
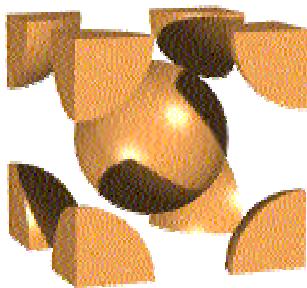


# Simple Cubic: unit cell

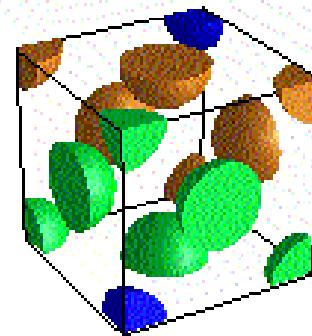
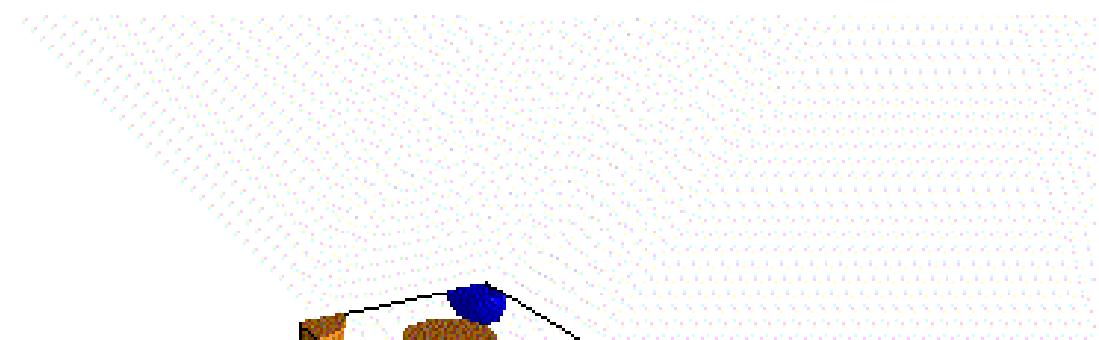
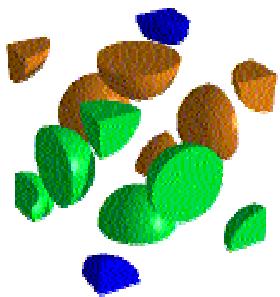


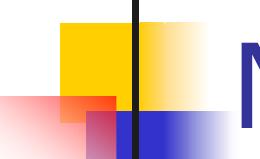


# Body Centered Cubic: unit cell

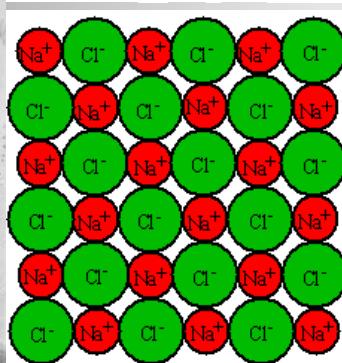
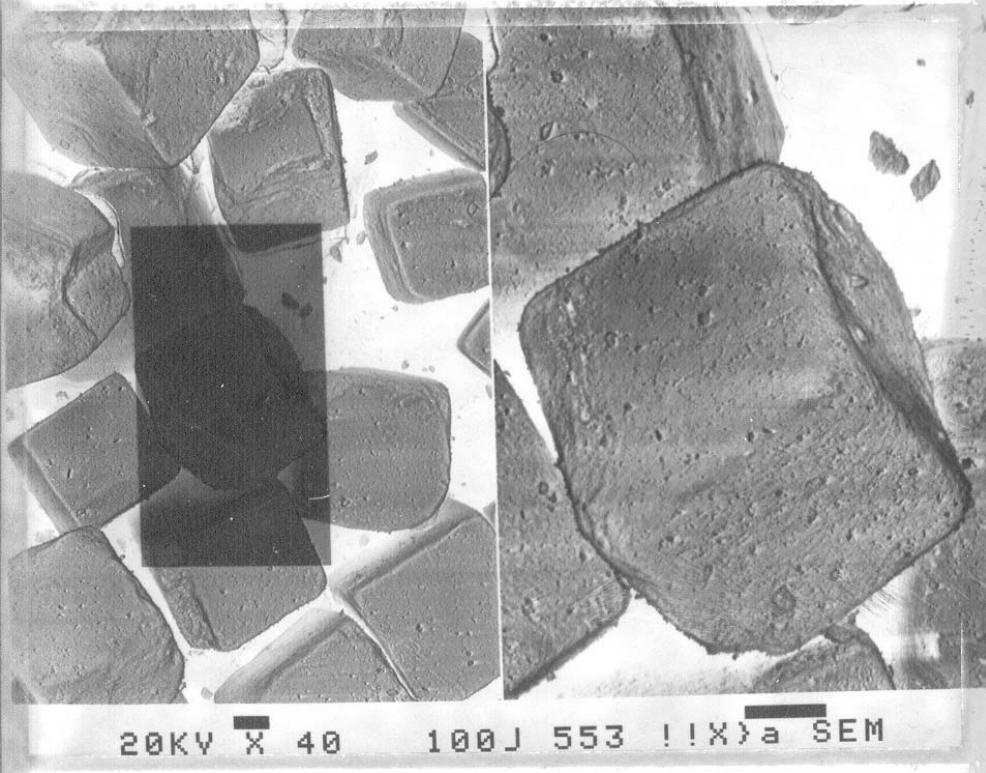


# Cubic Close Packed (FCC): unit cell

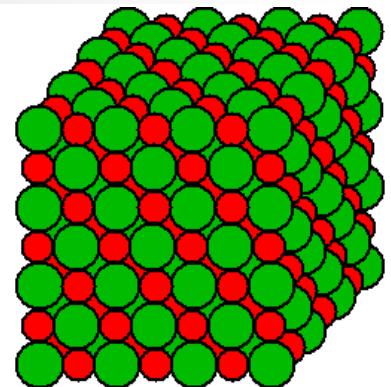




# NaCl (salt shaker variety)

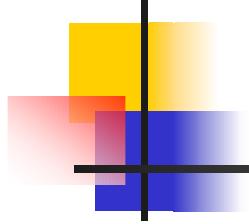


(a)

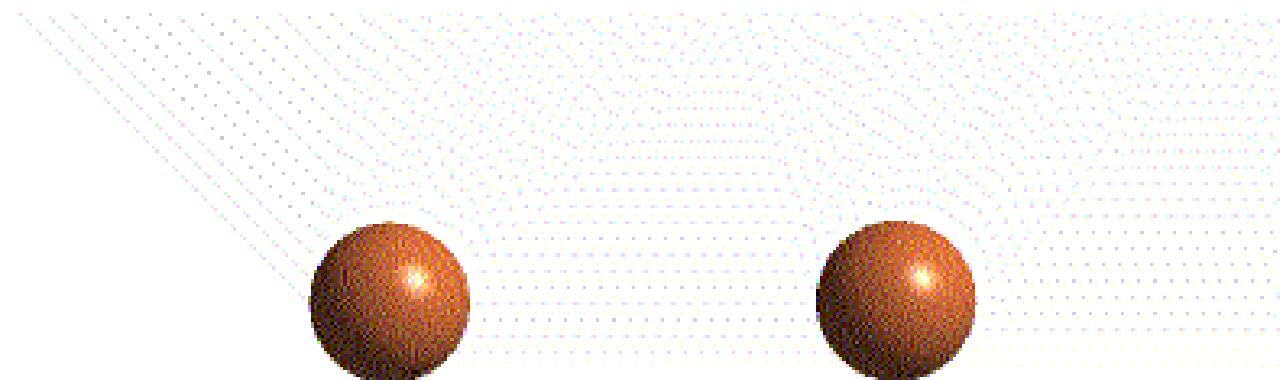
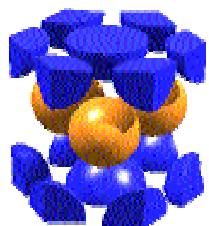


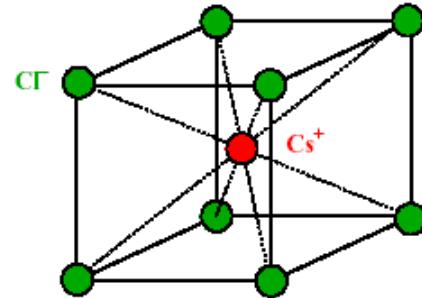
(b)

(a) A schematic illustration of a cross section from solid NaCl. NaCl solid is made of  $\text{Cl}^-$  and  $\text{Na}^+$  ions arranged alternately so that the oppositely charged ions are closest to each other and attract each other. There are also repulsive forces between the like-ions. In equilibrium the net force acting on any ion is zero. (b) Solid NaCl.

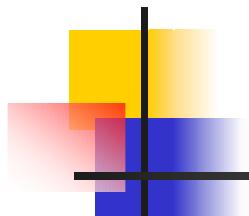


# Hexagonal Close Packed: unit cell

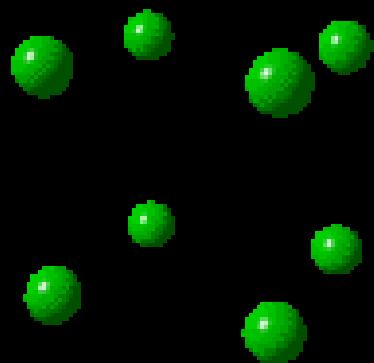
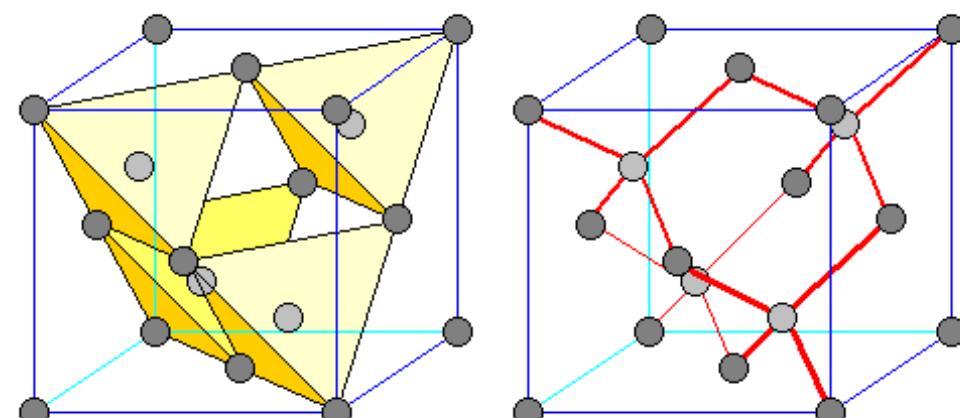


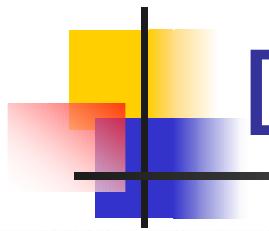


- Thinking about the unit cell as a three-dimensional graph allows us to describe the structure of a crystal with a remarkably small amount of information. We can specify the structure of cesium chloride, for example, with only four pieces of information.
  - CsCl crystallizes in a cubic unit cell.
  - The length of the unit cell edge is 0.4123 nm.
  - There is a Cl<sup>-</sup> ion at the coordinates 0,0,0.
  - There is a Cs<sup>+</sup> ion at the coordinates 1/2,1/2,1/2.
- Because the cell edge must connect equivalent lattice points, the presence of a Cl<sup>-</sup> ion at one corner of the unit cell (0,0,0) implies the presence of a Cl<sup>-</sup> ion at every corner of the cell. The coordinates 1/2,1/2,1/2 describe a lattice point at the center of the cell. Because there is no other point in the unit cell that is one cell-edge length away from these coordinates, this is the only Cs<sup>+</sup> ion in the cell. CsCl is therefore a simple cubic unit cell of Cl<sup>-</sup> ions with a Cs<sup>+</sup> in the center of the body of the cell.

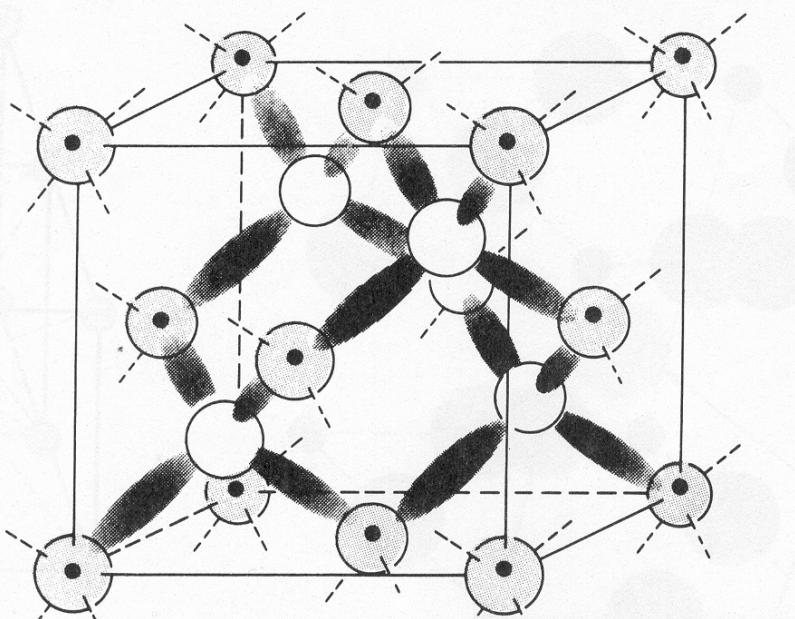
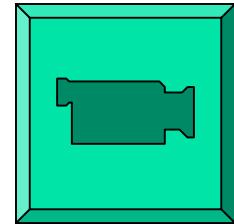


# Diamond

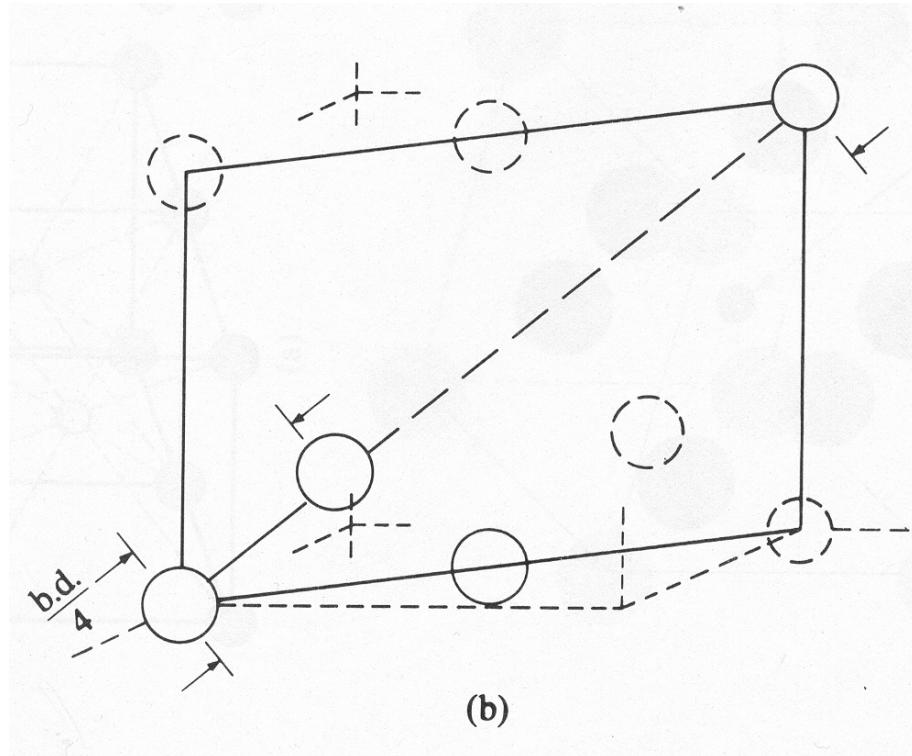




# Diamond cubic structure



(a)



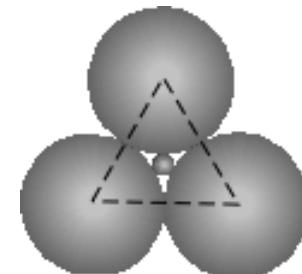
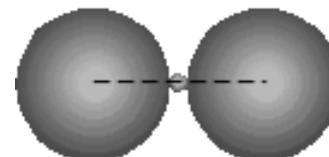
(b)

# Coordination number

- **coordination number:** the number of atoms closest to any given atom in a crystal.
  - The arrangement of atoms in a crystal structure not only depends on the charge on the ion and type of bonding between atoms, but also on the size of the atoms or ions.
  - In any given molecule or crystal structure each atom or ion will be surrounded by other atoms or ions. The number of ions or atoms that immediately surround an atom or ion of interest is called the **coordination number, - C.N.**
- As we shall see, the coordination number depends on the relative size of the atoms or ions. So, we must first discuss their sizes.

At values of  $R_x/R_z < 0.155$  the only way the smaller ion can be coordinated by the larger ions is to have 2 of the larger ions on either side. This 2-fold coordination is termed **linear coordination**.

For **triangular coordination**, the coordination number is three, that is 3 anions surround the smaller cation. The "no rattle" limit is reached for triangular coordination when  $R_x/R_z$  becomes less than 0.155.



# Coordination number

For  $R_x/R_z < 0.414$  the structure goes into 4-fold coordination. Planes through the centers of the larger atoms in this case will form a tetrahedron, so 4-fold coordination is also called **tetrahedral coordination**.

Six-fold coordination is also called **octahedral coordination** because the shape defined by drawing planes through the center of the larger ions is an octahedron. Octahedral coordination is stable when  $R_x/R_z > 0.732$ , but decreasing the radius of cation,  $R_x$ , will eventually reach a limit where again the smaller ion will rattle in its site.

The **no rattle limit** can be determined by looking at the horizontal plane running through the ions labeled C and D. In this case we can write:

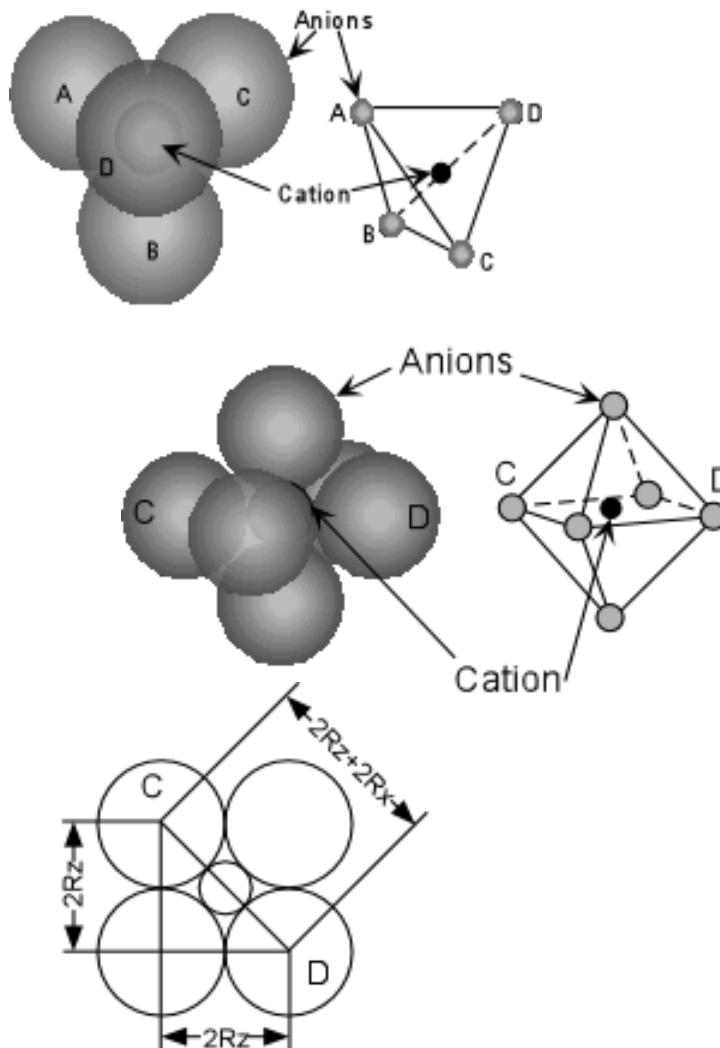
$$(2R_z + 2R_x)^2 = (2R_z)^2 + (2R_z)^2 = 2(4R_z^2)$$

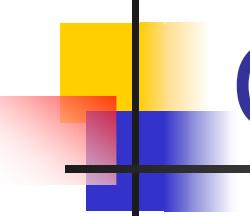
$$2R_z + 2R_x = 2\sqrt{2}R_z$$

$$R_z + R_x = \sqrt{2}R_z$$

$$R_x = (\sqrt{2} - 1)R_z$$

$$R_x/R_z = 0.414$$





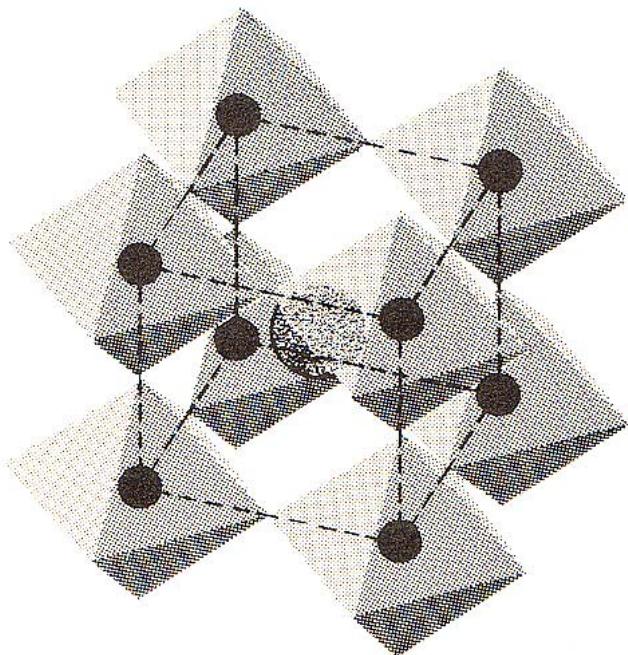
# Coordination Numbers

The table here summarizes the cation to anion radius ratios,  $R_x/R_z$ , for various coordination numbers and gives the name of the coordination polyhedron for each coordination number.

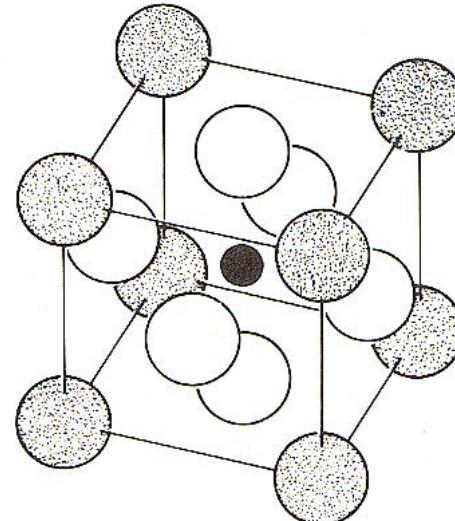
coord. number	radius ratio	exact	geometry
2	0.000-0.155	$0 \text{ to } \frac{2}{3}\sqrt{3} - 1$	linear
3	0.155-0.225	$\frac{2}{3}\sqrt{3} - 1 \text{ to } \frac{1}{2}\sqrt{6} - 1$	trigonal planar
4	0.225-0.414	$\frac{1}{2}\sqrt{6} - 1 \text{ to } \sqrt{2} - 1$	tetrahedral
6	0.414-0.732	$\sqrt{2} - 1 \text{ to } \sqrt{3} - 1$	octahedral
8	0.732-1.000	$\sqrt{3} - 1 \text{ to } 1$	cubic

The radius ratio limits are determined from geometry (Klein and Hurlbut 1985).

# Perovskite Structure $\text{CaTiO}_3$



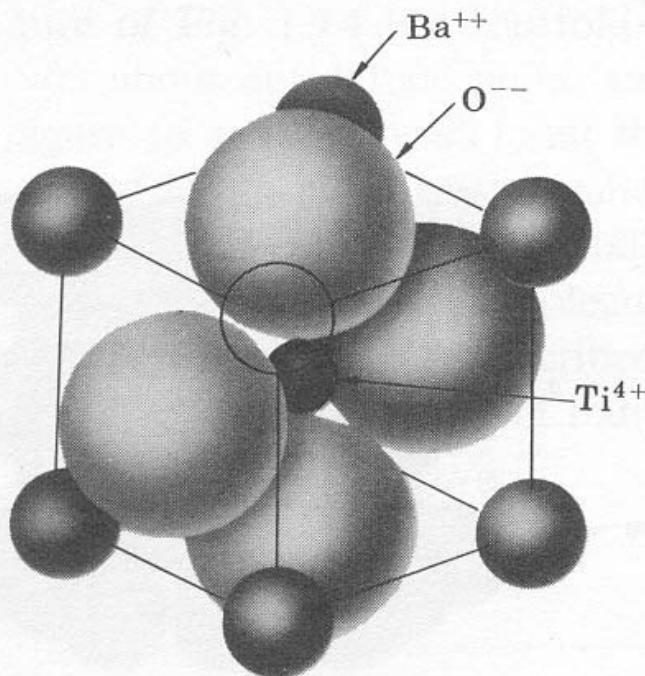
(a) Ti atoms at the corners of the unit cube<sup>3</sup>



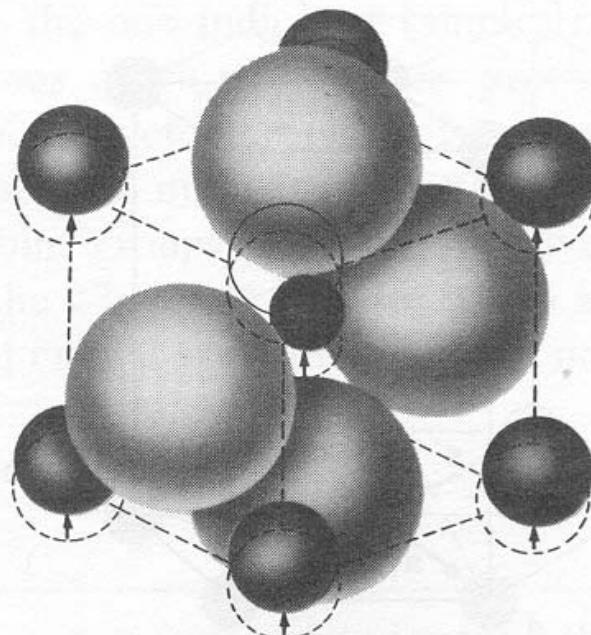
(b) Ti atoms in the center of the unit cube. Oxygen atoms at center of face, and Ca atoms at the corners

Perovskite structure ( $\text{CaTiO}_3$ ).

# Ferroelectric Barium Titanate: What happens when your marbles are loose

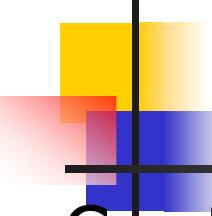


(a) Unpolarized  $\text{BaTiO}_3$  has a cubic structure and the cations touch each of the surrounding oxygen ions.



(b) Polarization develops when the cations move upwards relative to the oxygen ions.

Illustration of the changes in atomic arrangement that accompany the development of the ferroelectric state in barium titanate.



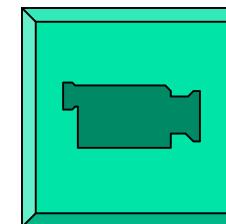
# Ceramics

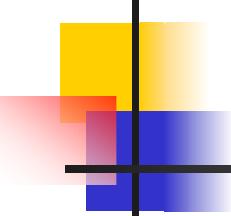
## ■ Crystal structures

- oxygen larger – generally in FCC lattice
- cations go in lattice sites based on
  - size
  - stoichiometry
  - charge balance
  - bond hybridization
- no good slip planes – brittle failure

## ■ Silicates

- built up of  $\text{SiO}_4^{4-}$
- layered
- counterions to neutralize charge

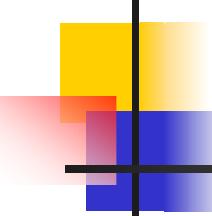




# Ceramics

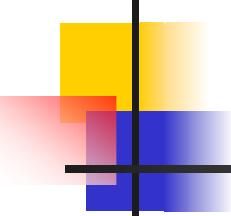
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- Carbon forms
  - diamond
  - graphite
  - fullerenes
  - amorphous
- Lattice imperfections
  - Frenkel defect – cation displaced into interstitial site
  - Schottky defect – missing cation/anion pair
- Phase diagrams
- Mechanical properties



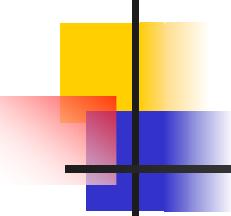
# Ceramics (cont)

- Glasses
  - amorphous sodium or borosilicates
  - Forming
    - pressing
    - drawing
    - blowing
- Clay products - forming
  - Hydroplastic forming
  - Slip casting
  - Refractories
  - Powder pressing
- Cements
- Advanced ceramics



# Atomic and Ionic Radii

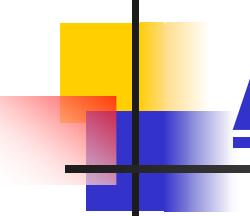
- The **size** of an atom or ion depends on the size of the nucleus and the number of electrons. Generally atoms with higher numbers of electrons have larger radii than those with smaller numbers of electrons.
- Thus ions will have radii different from the atoms because ions will have either gained or lost electrons.
- The **number** of positive charges in the nucleus determines both the number of electrons that surround an atom and the number of electrons that can be lost or gained to form ions.
  - Thus as the charge on the ion becomes more positive, there will be less electrons and the ion will have a smaller radius.
  - As the charge on the ion becomes more negative, there will be more electrons and the ion will have a larger radius.
- As the **atomic number increases** in any given column of the Periodic Table, the number of protons and electrons increases and thus the **size of the atom or ion increases**.
- Atomic and ionic radii also depend on the **type of bonding** that takes place between the constituents, and on the coordination number. Thus, atomic and ionic radii will vary somewhat as a function of the environment in which the atoms or ions are found.



# Metals atomic radii

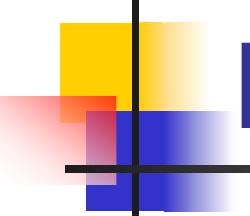
Atomic Radii and Crystal Structures for 16 Metals

Metal	Crystal Structure <sup>a</sup>	Atomic Radius <sup>b</sup> (nm)	Metal	Crystal Structure	Atomic Radius (nm)
Aluminum	FCC	0.1431	Molybdenum	BCC	0.1363
Cadmium	HCP	0.1490	Nickel	FCC	0.1246
Chromium	BCC	0.1249	Platinum	FCC	0.1387
Cobalt	HCP	0.1253	Silver	FCC	0.1445
Copper	FCC	0.1278	Tantalum	BCC	0.1430
Gold	FCC	0.1442	Titanium ( $\alpha$ )	HCP	0.1445
Iron ( $\alpha$ )	BCC	0.1241	Tungsten	BCC	0.1371
Lead	FCC	0.1750	Zinc	HCP	0.1332



# ATOMIC PACKING

How the atoms, ions, or molecules are arranged determines the properties of the particular crystal. The atomic packing factor or APF can be defined as the number of atoms occupying a given space. This can be applied to unit cells as well as planes.



# Number of atoms per unit cell

- If a metal crystallized in a simple cubic unit cell, there would be a metal atom on each of the eight corners of the cell. Because only one-eighth of these atoms can be assigned to a given unit cell, each unit cell in a simple cubic structure would have one net metal atom.

- *Simple cubic structure:*

$$8 \text{ corners} \times 1/8 = 1 \text{ atom}$$

- If a metal formed a body-centered cubic structure, there would be two atoms per unit cell, because the metal atom in the center of the body wouldn't be shared with any other unit cells.

- *Body-centered cubic structure:*

$$(8 \text{ corners} \times 1/8) + 1 \text{ body} = 2 \text{ atoms}$$

- If metal crystallized in a face-centered cubic structure, the six atoms on the faces of the unit cell would contribute three net metal atoms, for a total of four atoms per unit cell.

- *Face-centered cubic structure:*

$$(8 \text{ corners} \times 1/8) + (6 \text{ faces} \times 1/2) = 4 \text{ atoms}$$

- Because they have different numbers of atoms in a unit cell, each of these structures would have a different density. Let's therefore calculate the density for the metal based on each of these structures and the unit cell edge length for this metal is given as: 0.3524 nm. In order to do this, we need to know the volume of the unit cell in cubic centimeters and the mass of a single metal atom.

P.D. = # of atoms in the unit cell/volume of unit cell

## Volume packing/density

Because they have different numbers of atoms in a unit cell, each of these structures would have a different density. Let's therefore calculate the density for nickel based on each of these structures and the unit cell edge length for nickel given in the tables: 0.3524 nm. In order to do this, we need to know the volume of the unit cell and the mass of a single nickel atom.

The volume ( $V$ ) of the unit cell is equal to the cell-edge length ( $a$ ) cubed.

$$V = a^3 = (0.3524 \text{ nm})^3 = 0.04376 \text{ nm}^3$$

Since there are  $10^9$  nm in a meter and 100 cm in a meter, there must be  $10^7$  nm in a cm.

$$\frac{10^9}{1 \text{ m}} \times \frac{1 \text{ m}}{100 \text{ cm}} = 10^7 \text{ nm/cm}$$

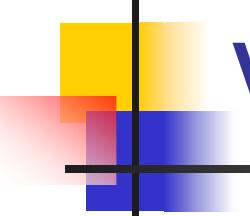
We can therefore convert the volume of the unit cell to  $\text{cm}^3$  as follows.

$$4.376 \times 10^{-23} \text{ nm}^3 \times \left[ \frac{1 \text{ cm}}{10^7 \text{ nm}} \right]^3 = 4.376 \times 10^{-23} \text{ cm}^3$$

The mass of a nickel atom can be calculated from the atomic weight of this metal and Avogadro's number.

$$\frac{58.69 \text{ g/mol}}{1 \text{ mol}} \times \frac{1 \text{ mol}}{6.022 \times 10^{23} \text{ atoms}} = 9.746 \times 10^{-23} \text{ g/atom} \quad \frac{9.746 \times 10^{-23} \text{ g/unit cell}}{4.376 \times 10^{-23} \text{ cm}^3/\text{unit cell}} = 2.23 \text{ g/cm}^3$$

The density of nickel, if it crystallized in a simple cubic structure, would therefore be  $2.23 \text{ g/cm}^3$ , to three significant figures.



# Volume packing/density

Because there would be twice as many atoms per unit cell if nickel crystallized in a body-centered cubic structure, the density of nickel in this structure would be twice as large.

*Body-centered cubic structure:*

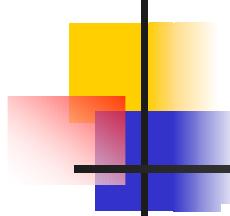
There would be four atoms per unit cell in a face-centered cubic structure and the density of nickel in this structure would be four times as large.

$$\frac{2(9.746 \times 10^{-23} \text{ g/unit cell})}{4.376 \times 10^{-23} \text{ cm}^3/\text{unit cell}} = 4.45 \text{ g/cm}^3$$

*Face-centered cubic structure:*

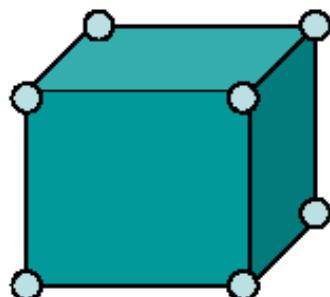
The experimental value for the density of nickel is 8.90 g/cm<sup>3</sup>. The obvious conclusion is that nickel crystallizes in a face-centered cubic unit cell and therefore has a cubic closest-packed structure.

$$\frac{4(9.746 \times 10^{-23} \text{ g/unit cell})}{4.376 \times 10^{-23} \text{ cm}^3/\text{unit cell}} = 8.91 \text{ g/cm}^3$$



# SC Lattice

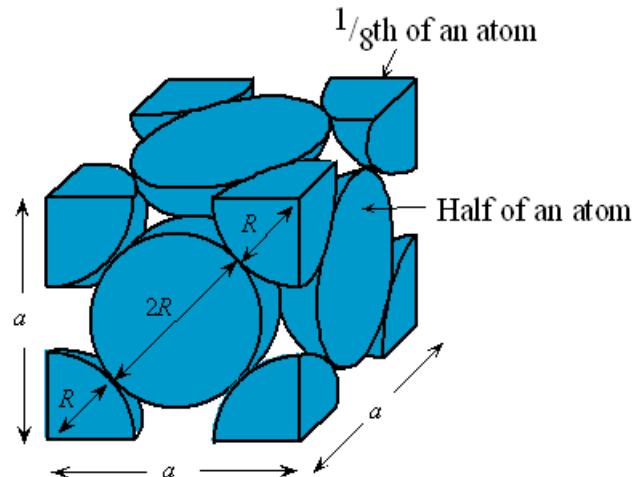
## Simple Cubic Lattice



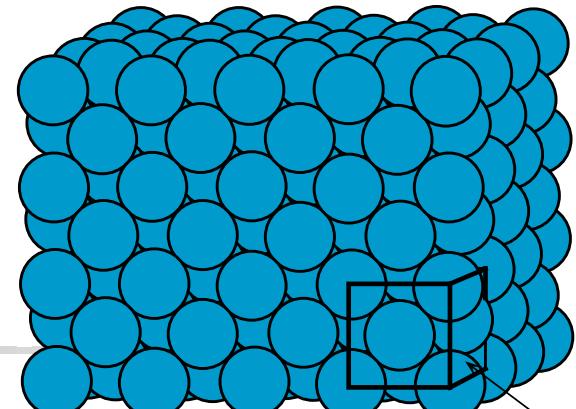
- 1) Close-pack relationship between the lattice parameter (a) and the atomic radius ( $r$ )  
 $\rightarrow a = 2r$
- 2) Coordination Number (CN) = 6
- 3) Unit Cell Density
- 4) Atomic Packing Factor = 0.52

$$\frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}}$$

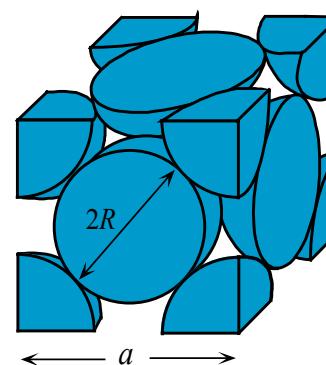
# FCC Unit Cell



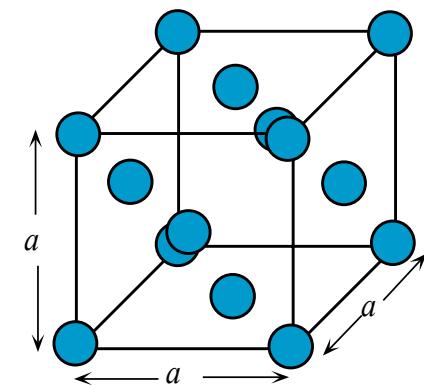
The FCC unit cell. The atomic radius is  $R$  and the lattice parameter is  $a$



(a)



(b)

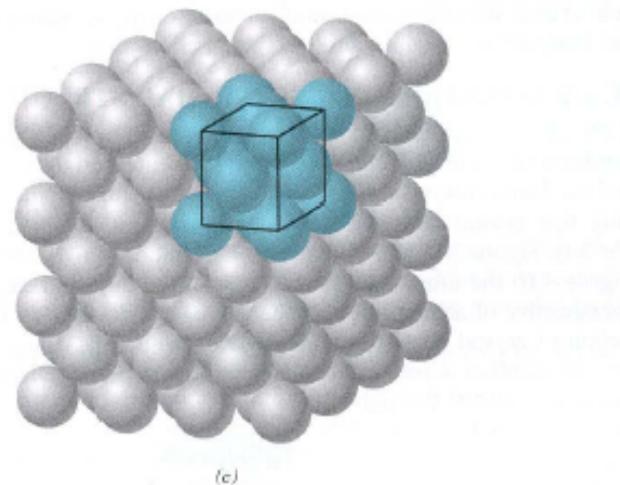
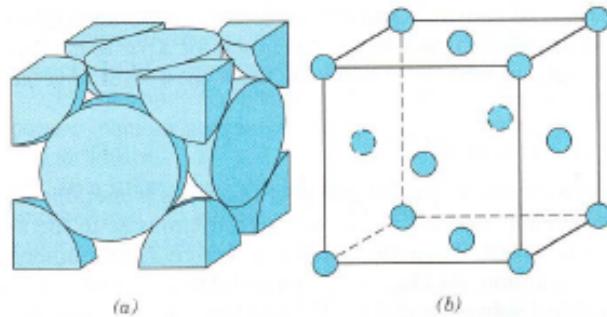


(c)

(a) The crystal structure of copper is Face Centered Cubic (FCC). The atoms are positioned at well defined sites arranged periodically and there is a long range order in the crystal. (b) An FCC unit cell with closed packed spheres. (c) Reduced sphere representation of the FCC unit cell. Examples: Ag, Al, Au, Ca, Cu,  $\gamma$ -Fe ( $>912^{\circ}\text{C}$ ), Ni, Pd, Pt, Rh

# FCC Lattice

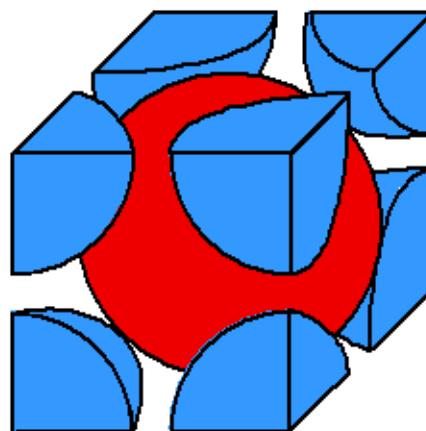
## Face-Centered Cubic Lattice



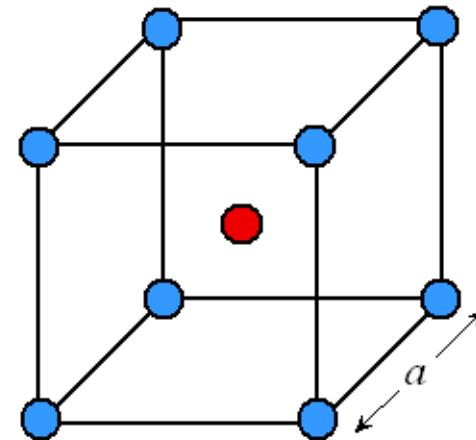
- 1) Close-pack relationship between the lattice parameter ( $a$ ) and the atomic radius ( $r$ )  $\rightarrow a = 2r\sqrt{2}$
- 2) Coordination Number (CN) = 12
- 3) Unit Cell Density
- 4) Atomic Packing Factor = 0.74

$$\frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}}$$

# BCC Unit Cell



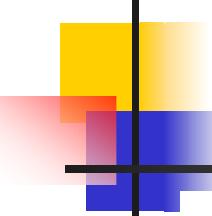
a



b

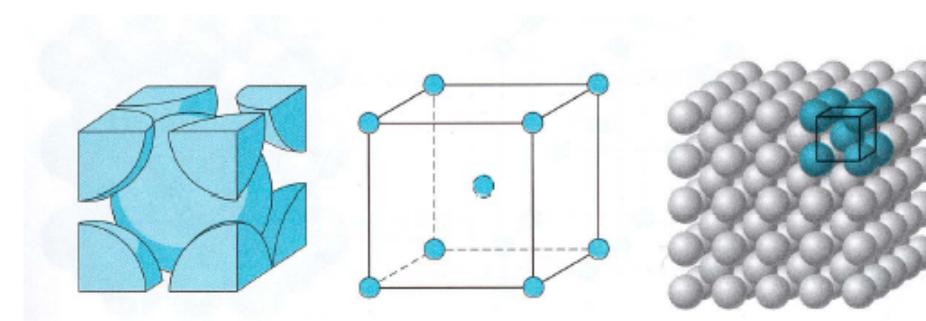
Examples: Alkali metals (Li, Na, K, Rb), Cr, Mo, W, Mn,  $\alpha$ -Fe ( $< 912^{\circ}\text{C}$ ),  $\beta$ -Ti ( $> 882^{\circ}\text{C}$ ).

Body centered cubic (BCC) crystal structure. (a) A BCC unit cell with closely packed hard spheres representing the Fe atoms. (b) A reduced-sphere unit cell.



# BCC Lattice

## Body-Centered Cubic Lattice

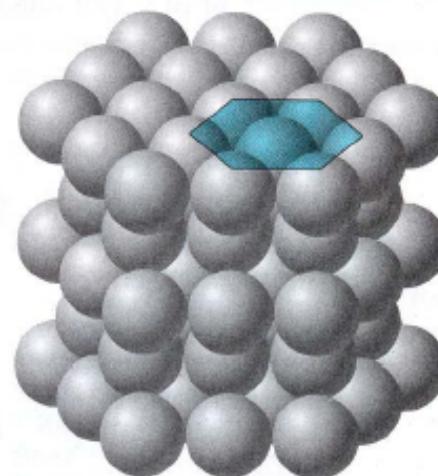
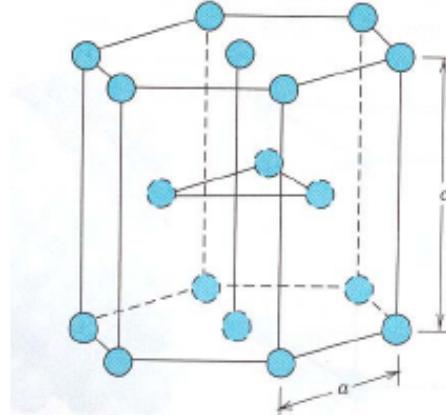


- 1) Close-pack relationship between the lattice parameter ( $a$ ) and the atomic radius ( $r$ )  $\rightarrow 4r = \sqrt{3} a$
- 2) Coordination number: 8
- 3) Unit Cell Density
- 4) Atomic packing factor is: 0.68

$$\frac{\text{volume of atoms in a unit cell}}{\text{total unit cell volume}}$$

# HCP Lattice

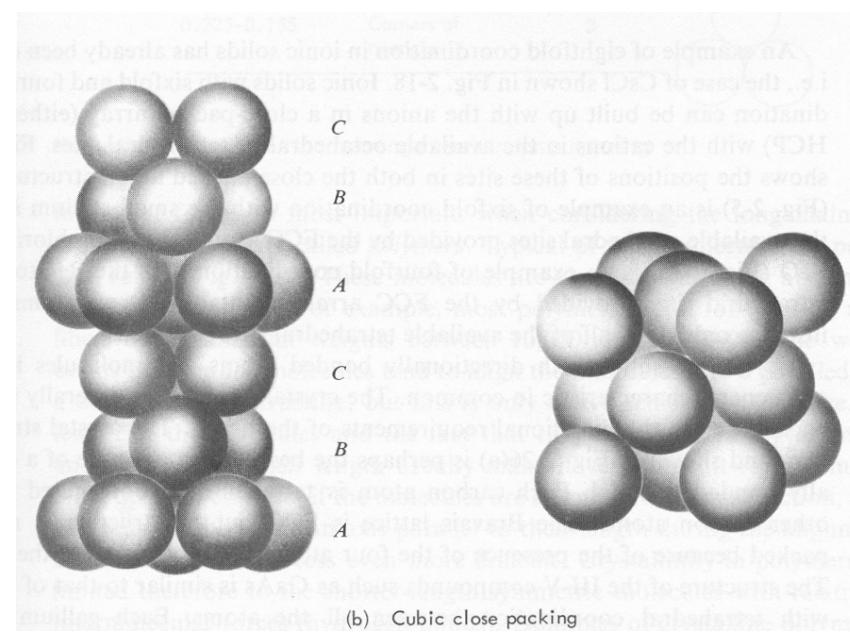
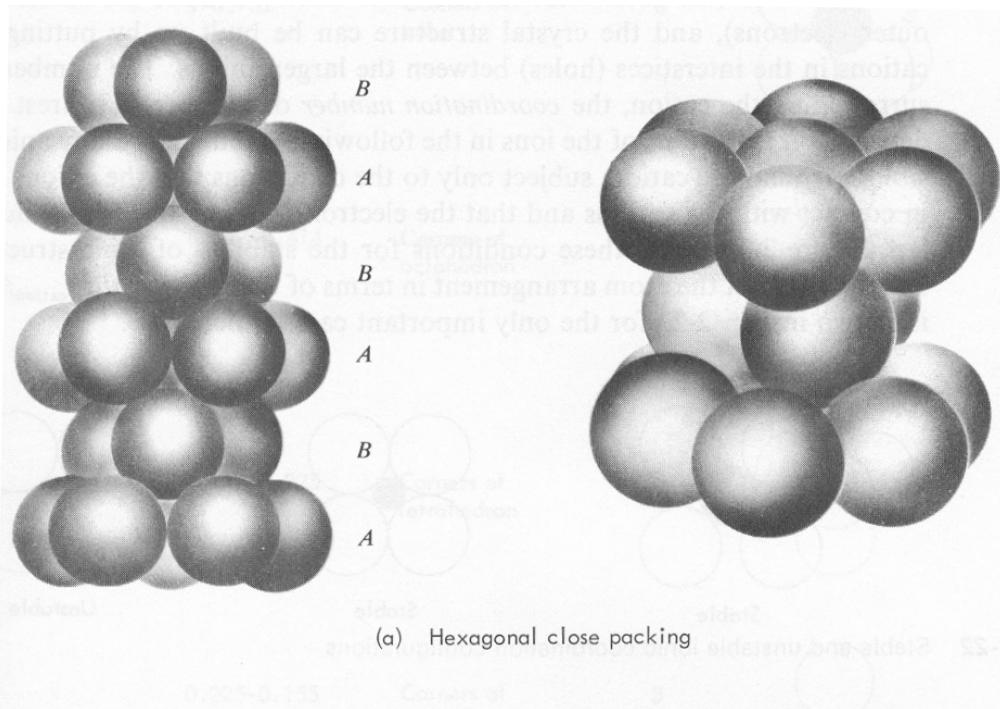
## Hexagonal Close-Packed Lattice



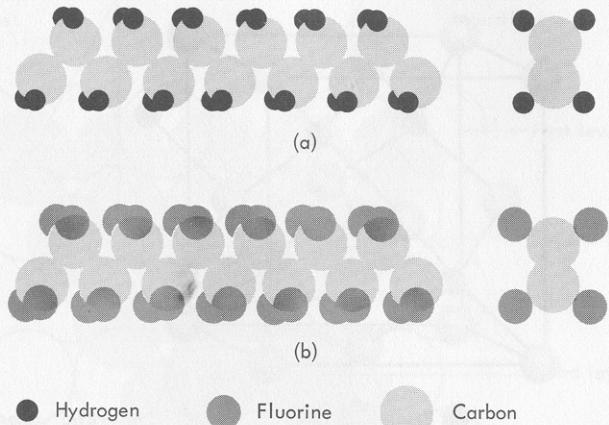
Coordination number: 12

Atomic packing factor is: 0.74

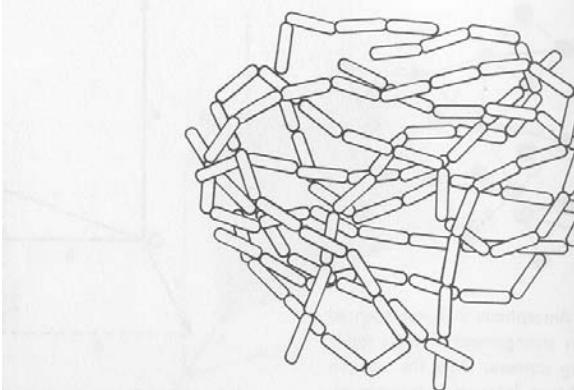
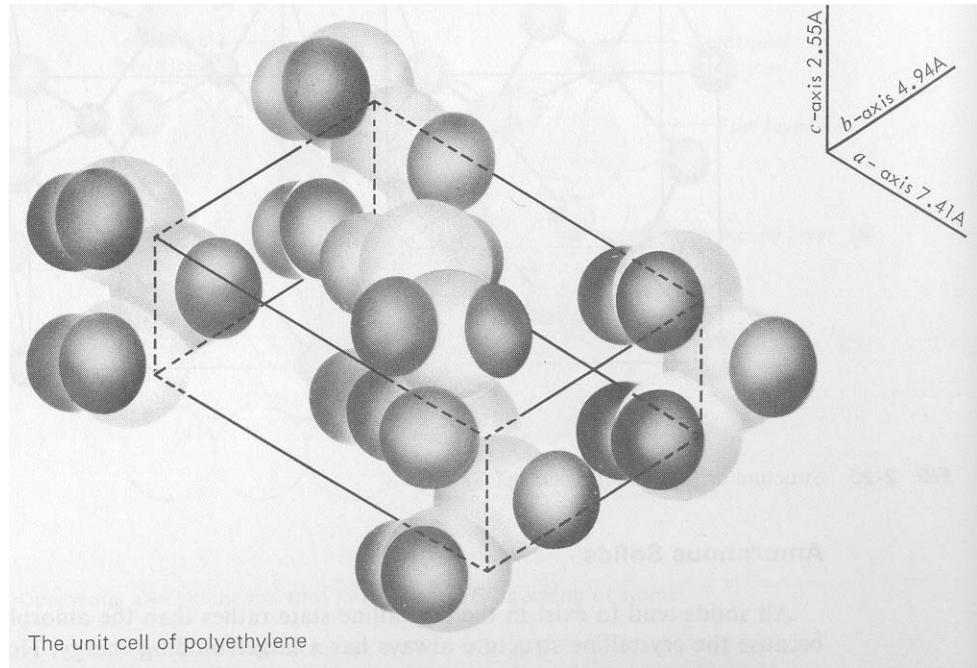
# Stacking/Packing Sequence for (a) HCP and (b) FCC



# Polymers



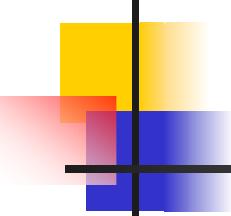
Atom arrangements in polymer chains of (a) polyethylene and (b) polytetrafluoroethylene (Teflon).



A schematic representation of a long-chain polymer. Each segment is one of the repeating units of the polymer chain.

# Properties of some important crystal structures

Crystal Structure	$a$ and $R$ ( $R$ is the radius of the atom).	Coordination Number (CN)	Number of atoms per unit cell	Atomic Packing Factor	Examples
Simple cubic	$a = 2R$	6 for ach atom	1	0.52	CsCl (2 at./u.c., 1 for each at. on its own cubic lattice)
BCC	$a = 4R/\sqrt{3}$	8	2	0.68	Many metals: $\alpha$ -Fe, Cr, Mo, W
FCC	$a = 4R/\sqrt{2}$	12	4	0.74	Many metals Ag, Au, Cu, Pt
HCP	$a = 2R$ $c = 1.633a$	12	2	0.74	Many metals: Co, Mg, Ti, Zn
Diamond	$a = 8R/\sqrt{3}$	4	8	0.34	Covalent solids: Diamond, Ge, Si, $\alpha$ -Sn.
Zinc blende		4	8	0.34	Many covalent and ionic solids. Many compound semiconductors. ZnS, GaAs, GaSb, InAs, InSb
NaCl		6	4 cations 4 anions	0.67 (NaCl)	Ionic solids such as NaCl, AgCl, LiF MgO, CaO Ionic packing factor depends on relative sizes of ions.
CsCl		8	1 cation 1 anion		Ionic solids such as CsCl, CsBr, CsI



# Examples

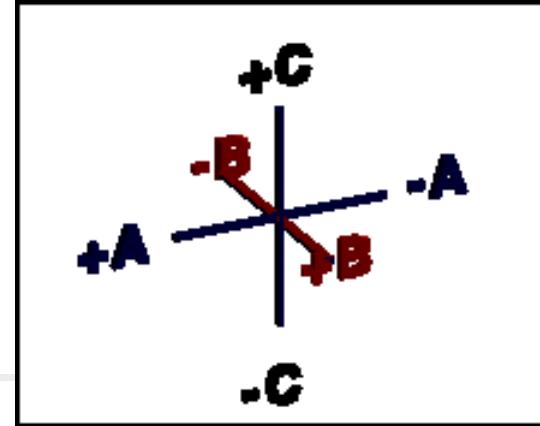
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## Example: Metallic Crystal Systems

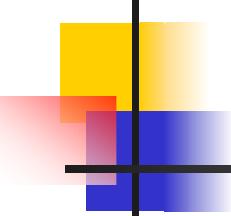
Find the lattice parameter of BCC Iron (Fe).

The lattice parameter of Palladium (Pd) is 0.38908 nm. Its atomic radius is 0.1376 nm. What is the lattice structure of Palladium? Assume Pd belongs to the cubic lattice system.

# Miller indices



- The Miller indices are referenced to the crystallographic axes of a crystal. They therefore do not have to be oriented at right angles (and are not for monoclinic and triclinic crystals). For orthorhombic crystals, there is unfortunately no convention on how to define the  $a$  axis.
- The Miller indices are found by determining the points at which a given crystal plane intersects the three axes, say at  $(a,0,0)$ ,  $(0,b,0)$ , and  $(0,0,c)$ . **If the plane is parallel an axis, it is given an intersection  $\infty$ .**
- The Miller index for the face is then specified by  $(1/a \ 1/b \ 1/c)$ , where the three numbers are expressed as the smallest integers, and negative quantities are indicated with an overbar.
- A face, when given with the crystal class, determines a set of faces known as a form and is denoted  $\{a \ b \ c\}$ . The vector normal to a face is specified as  $[a \ b \ c]$ , and the family of normals as  $\langle a \ b \ c \rangle$ .

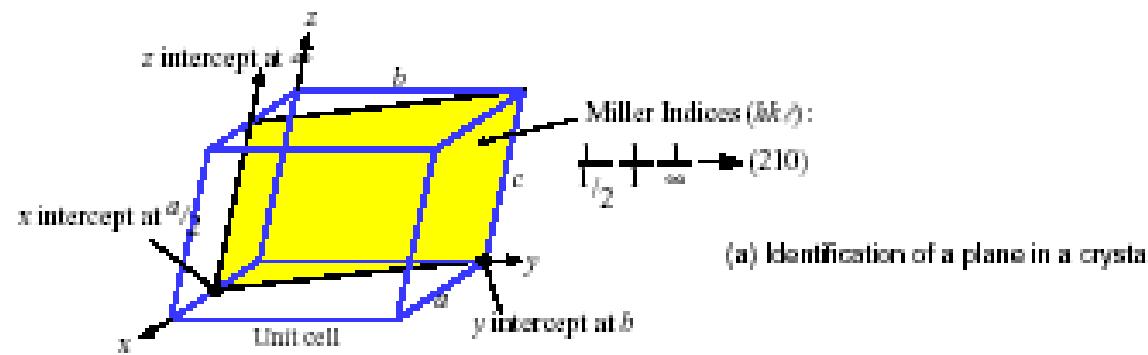


# Crystallographic Planes

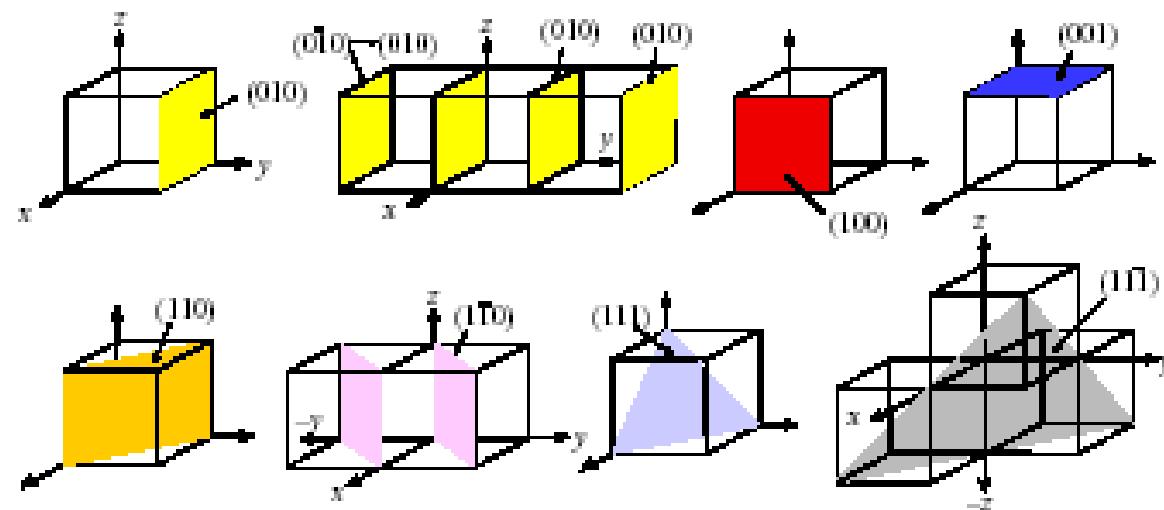
The orientations of planes for a crystal structure are represented in a similar manner. Again, the unit cell is the basis, with the three-axis coordinate system as represented in Figure 3.4. In all but the hexagonal crystal system, crystallographic planes are specified by three Miller indices as  $(hkl)$ . Any two planes parallel to each other are equivalent and have identical indices. The procedure employed in determination of the  $h$ ,  $k$ , and  $l$  index numbers is as follows:

1. If the plane passes through the selected origin, either another parallel plane must be constructed within the unit cell by an appropriate translation, or a new origin must be established within the unit cell by an appropriate translation, or a new origin must be established at the corner of another unit cell.
2. At this point the crystallographic plane either intersects or parallels each of the three axes; the length of the planar intercept for each axis is determined in terms of the lattice parameters  $a$ ,  $b$ , and  $c$ .
3. The reciprocals of these numbers are taken. A plane that parallels an axis may be considered to have an infinite intercept and, therefore, a zero index.
4. If necessary, these three numbers are changed to the set of smallest integers by multiplication or division by a common factor.
5. Finally, the integer indices, not separated by commas, are enclosed within parentheses, thus:  $(hkl)$ .

# Planes in a lattice

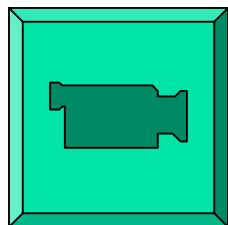


(a) Identification of a plane in a crystal



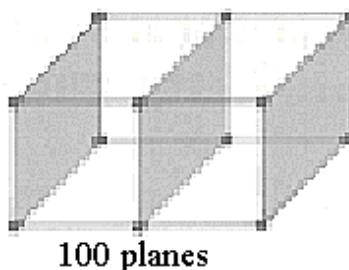
(b) Various planes in the cubic lattice

# Miller Indices for Cubic Lattice Planes

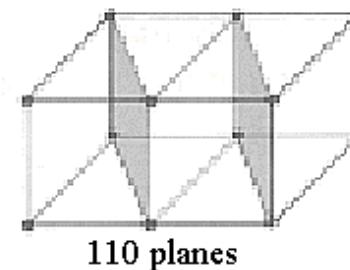


110 family

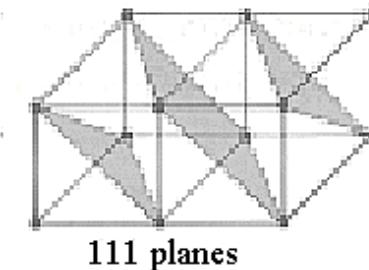
**Primitive  
cubic lattice**



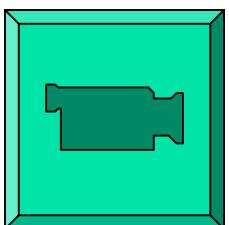
100 planes



110 planes

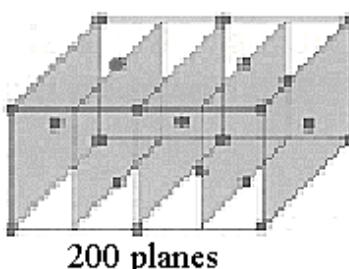


111 planes

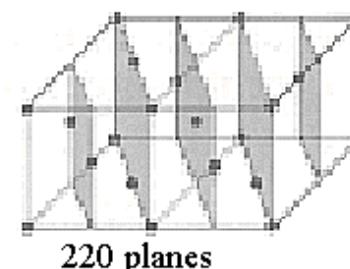


111 family

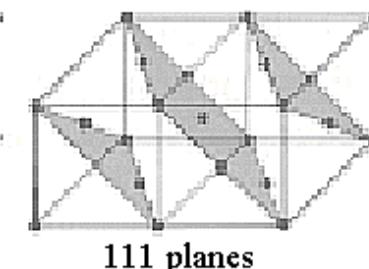
**Face-centred  
cubic lattice**



200 planes

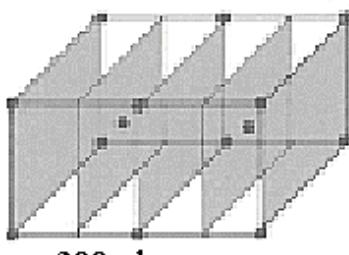


220 planes

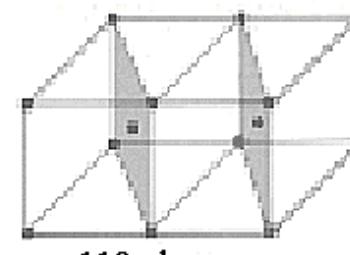


111 planes

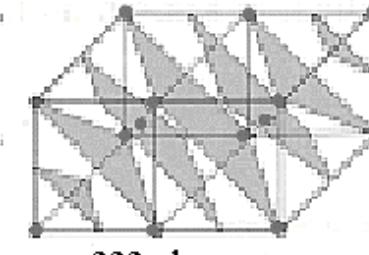
**Body-centred  
cubic lattice**



200 planes



110 planes



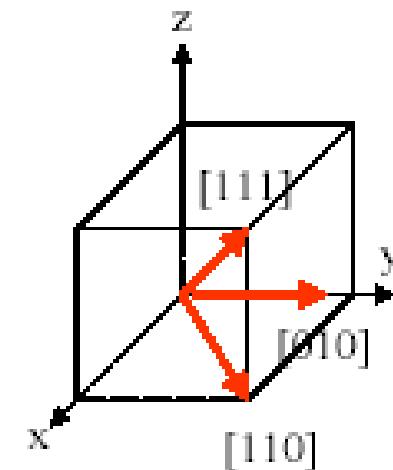
222 planes

Miller indices for three types of cubic lattices.

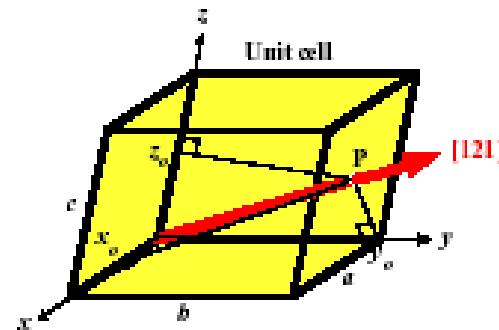
# Crystallographic Directions

A crystallographic direction is defined as a line between two points, or a vector. The following steps are utilized in the determination of the three directional indices:

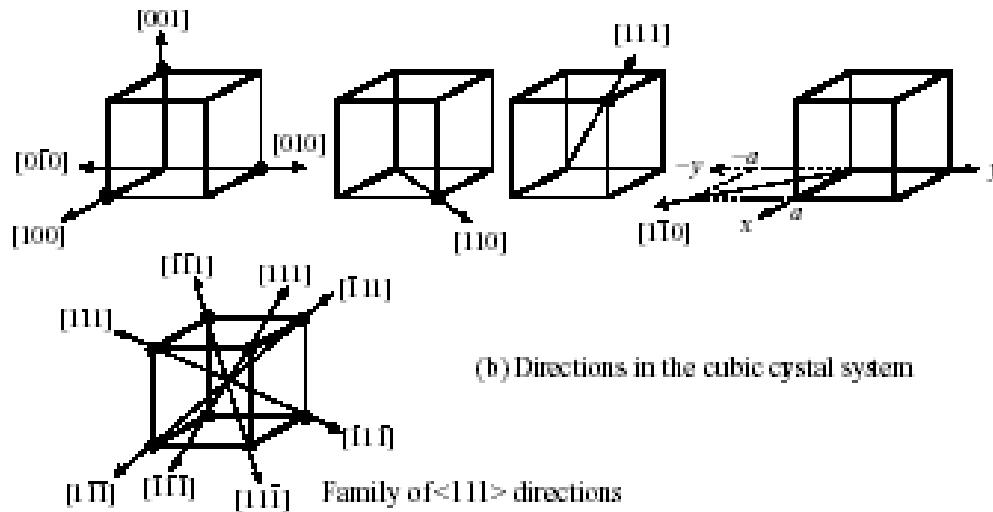
1. A vector of convenient length is positioned such that it passes through the origin of the coordinate system. Any vector may be translated throughout the crystal lattice without alteration, if parallelism is maintained.
2. The length of the vector projection on each of the three axes is determined; these are measured in terms of the unit cell dimensions  $a$ ,  $b$ , and  $c$ .
3. These three numbers are multiplied or divided by a common factor to reduce them to the smallest integer values.
4. The three indices, not separated by commas, are enclosed in square brackets, thus:  $[uvw]$ . The  $u$ ,  $v$ , and  $w$  integers correspond to the reduced projections along the  $x$ ,  $y$ , and  $z$  axes, respectively.



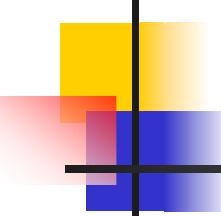
# Directions in a lattice



(a) Identification of a direction in a crystal.



(b) Directions in the cubic crystal system



# Interplanar spacing

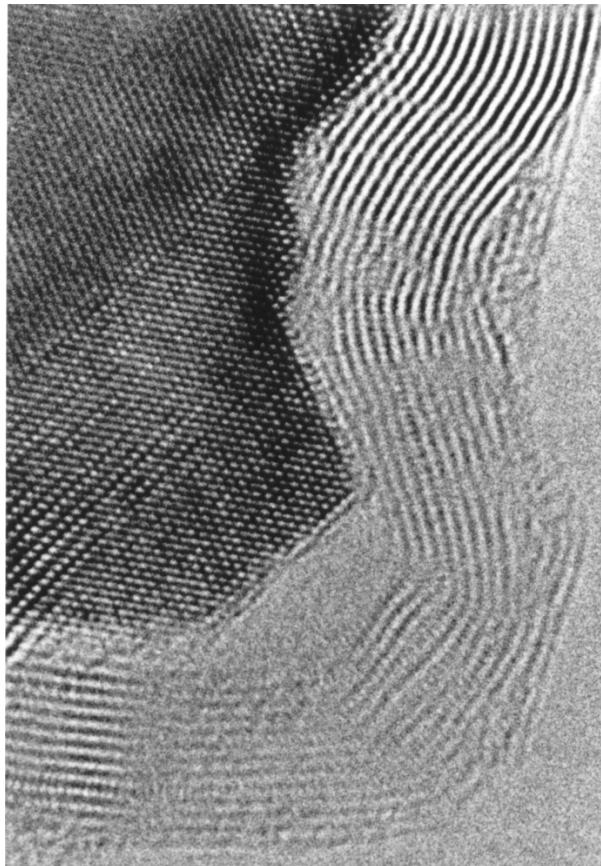
Only certain atomic planes in a given crystal structure will diffract electrons or X rays. The interplanar spacings between parallel planes are determined from the diffraction patterns and the lattice constants computed. For example, the interplanar spacing between  $hkl$  planes,  $d_{hkl}$ , for the orthorhombic system is related to the lattice parameters  $a$ ,  $b$ , and  $c$  by

$$\frac{1}{(d_{hkl})^2} = \left(\frac{h}{a}\right)^2 + \left(\frac{k}{b}\right)^2 + \left(\frac{l}{c}\right)^2$$

For the cubic system,  $a = b = c$ . By knowing the lattice parameters and the number and arrangement of atoms per cell, interatomic distances can be computed.

The spatial arrangement of atoms is also determined by X-ray-, electron-, and neutron-diffraction techniques. Here, a quantitative measure of the intensities of the rays reflected from the planes is required. Electron density maps or distributions for a given crystal plane can be synthesized from the experimentally determined intensities of diffracted X rays from a crystal, and effective *atomic radii* can be determined.

# Boron Nitride Layer on Magnesium Oxide

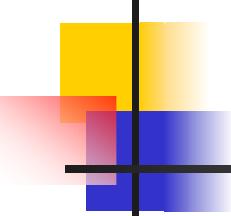


- 7,200,000 X Magnification.
- What is the interplanar spacing for Boron Nitride? For MgO?

# d-spacings for other crystals

Proportionality of the ratios of the radii of ring patterns for different crystal structures

Crystal structure	Formula for interplanar spacing	Possible values of $h$ , $k$ , $l$ for reflection (up to 20)	Criterion
simple cubic	$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2} = \frac{N}{a^2}$	$N$ an integer except 7 or 15	ratios of squares of radii $\propto N$
f.c.c.	$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2} = \frac{N}{a^2}$	$N = 3, 4, 8, 11, 12, 16, 19, 20$	ratios $\propto N$
b.c.c.	$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2} = \frac{N}{a^2}$	$N = 2, 4, 6, 8, 10, 12, 14, 16, 18, 20$	ratios $\propto N$
diamond structure	$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2} = \frac{N}{a^2}$	$N = 2, 8, 11, 16, 19$	ratios $\propto N$
tetragonal	$\frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$	$h^2 + k^2 = 1, 2, 4, 5, 8, 9, 10, 13, 16, 17, 18, 20$	ratios frequently proportional to 2; use Bunn chart, see Henry et al. (1951)
hexagonal	$\frac{1}{d^2} = \frac{4h^2 + hk + k^2}{3a^2} + \frac{l^2}{c^2}$	$h^2 + hk + k^2 = 1, 3, 4, 7, 9, 12, 13, 16, 19$	ratios frequently proportional to 3; use Bunn chart, see Henry et al. (1951)



# Example interplanar spacing

**Example** The intermetallic compound FeSi is cubic with four formula units per cell, and  $d_{321} = 1.1997 \text{ \AA}$  at 25°C. Compute the lattice constant and density of FeSi.

*Solution.*

$$\frac{1}{(d_{hkl})^2} = \left(\frac{h}{a}\right)^2 + \left(\frac{k}{b}\right)^2 + \left(\frac{l}{c}\right)^2$$

For the cubic system,  $a = b = c$ :

$$\frac{1}{(d_{hkl})^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

$$\frac{1}{(d_{321})^2} = \frac{3^2 + 2^2 + 1^2}{a^2}$$

$$a^2 = 14(d_{321})^2$$

$$a = \sqrt{14} (1.1997 \text{ \AA})$$

$$= 4.5 \text{ \AA} = 4.5 \times 10^{-10} \text{ m}$$

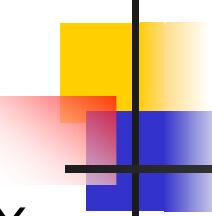
The molecular weight of FeSi is 83.94 kg/kg mol. Density is mass divided by volume.

$$\begin{aligned} \text{Density} &= 4 \times 83.94 \frac{\text{kg}}{\text{kg mol}} \times \frac{\text{kg mol}}{(6.02 \times 10^{26})} \times \frac{1}{(4.5 \times 10^{-10} \text{ m})^3} \\ &= 6.13 \times 10^3 \text{ kg/m}^3 \end{aligned}$$

# Interplanar angle

In general for any orthogonal system:

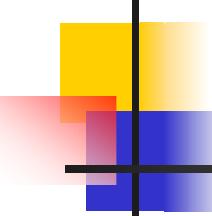
$$\cos \theta = \frac{h_1^2/a_1^2 + k_1^2/a_2^2 + l_1^2/a_3^2}{\sqrt{\left(\frac{h_1}{a_1}\right)^2 + \left(\frac{k_1}{a_2}\right)^2 + \left(\frac{l_1}{a_3}\right)^2} \sqrt{\left(\frac{h_2}{a_1}\right)^2 + \left(\frac{k_2}{a_2}\right)^2 + \left(\frac{l_2}{a_3}\right)^2}}$$



# X-Ray Analytical Methods

X-rays were discovered by W.C. Röentgen in 1895;  
led to three major uses:

- X-ray **radiography** is used for creating images of light-opaque materials relies on the relationship between density of materials and absorption of x-rays. Applications include a variety of medical and industrial applications.
- X-ray **fluorescence** spectrometry relies on characteristic secondary radiation emitted by materials when excited by a high-energy x-ray source and is used primarily to determine amounts of particular elements in materials.
- X-ray **crystallography** relies on the dual wave/particle nature of x-rays to discover information about the structure of crystalline materials.



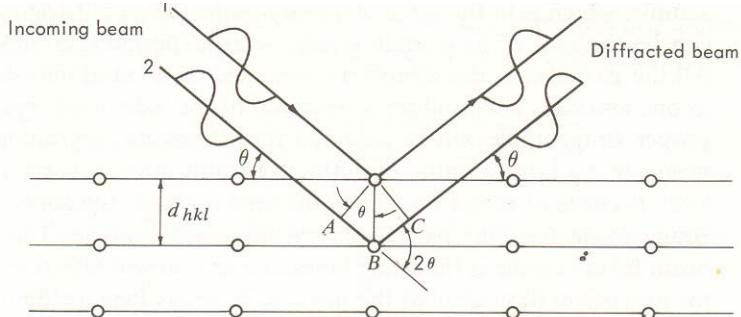
# Right tool, right job

Scatterers (spacings)	Radiation (typical dimension)
Ink dots in newsprint (0.1 mm)	Thermal radiation (0.1 nm typical)
Raindrops (10 mm)	Light (520 nm for green)
Row of parked cars (3 m)	Sound (1.26 m at middle C)
Precipitates in alloys (100 nm)	X-ray (0.154 nm for Cu K $\alpha$ )
Atoms in crystals (0.1 nm)	Electron-beam (3.7 pm for 100 keV)

# Bragg's Law and Diffraction: How waves reveal the atomic structure of crystals

- Bragg's Law refers to the simple equation:

$$n\lambda = 2d_{hkl} \sin\theta$$

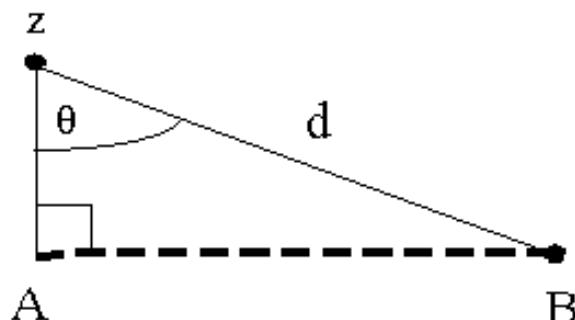
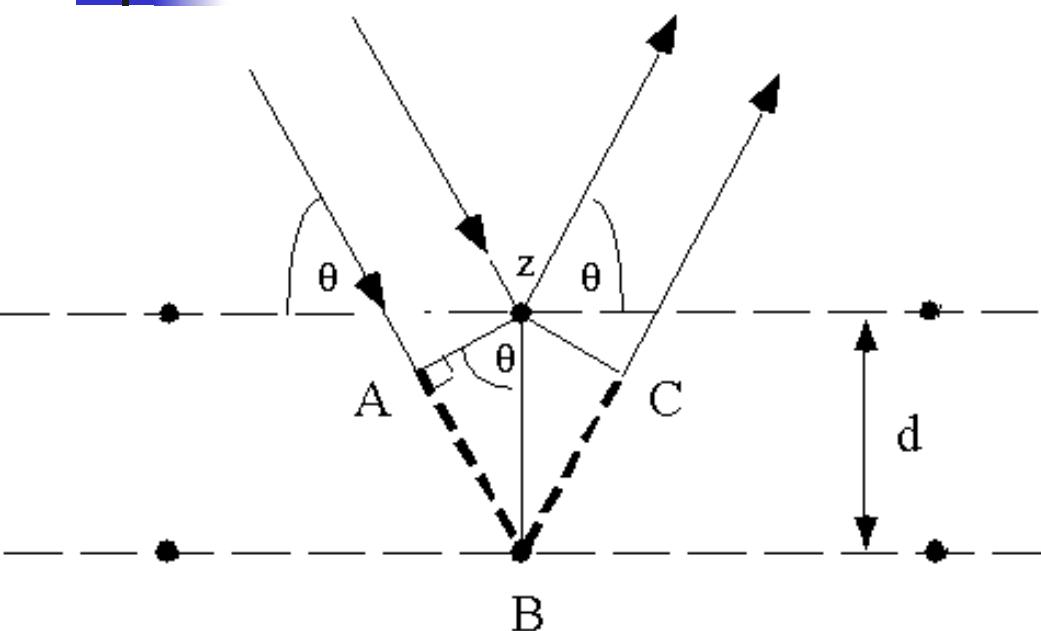


Derivation of Bragg's law, assuming the planes of atoms behave as reflecting planes

- derived by the English physicists Sir W.H. Bragg and his son Sir W.L. Bragg in 1913 to explain why the cleavage faces of crystals appear to reflect X-ray beams at certain angles of incidence (theta,  $\theta$ ). The variable  $d_{hkl}$  is the distance between atomic layers in the hkl plane of a crystal, and the variable lambda  $\lambda$  is the **wavelength** of the incident X-ray beam; n is an integer (the order of the interference).

- This observation is an example of X-ray **wave interference** (Roentgenstrahlinterferenzen), commonly known as X-ray diffraction (XRD), and was direct evidence for the periodic atomic structure of crystals postulated for several centuries. The Braggs were awarded the Nobel Prize in physics in 1915 for their work in determining crystal structures beginning with NaCl, ZnS and diamond. Although Bragg's law was used to explain the interference pattern of X-rays scattered by crystals, diffraction has been developed to study the structure of all states of matter with any beam, e.g., ions, electrons, neutrons, and protons, with a wavelength similar to the distance between the atomic or molecular structures of interest.

# Deriving Bragg's Law: constructive interference



The lower beam must travel the extra distance ( $AB + BC$ ) to continue traveling parallel and adjacent to the top beam. Recognizing  $d$  as the hypotenuse of the right triangle  $ABz$ , we can use trigonometry to relate  $d$  and  $\lambda$  to the distance ( $AB + BC$ ). The distance  $AB$  is opposite so,

$$AB = d \sin \theta .$$

Because  $AB = BC$ ,

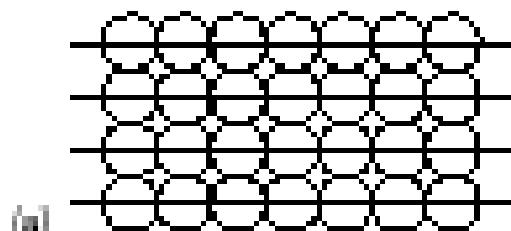
$$n\lambda = 2AB$$

Substituting we have,

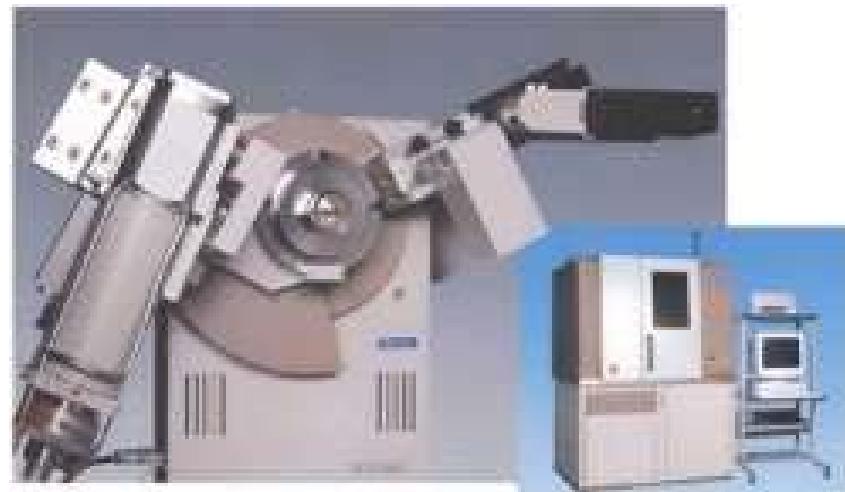
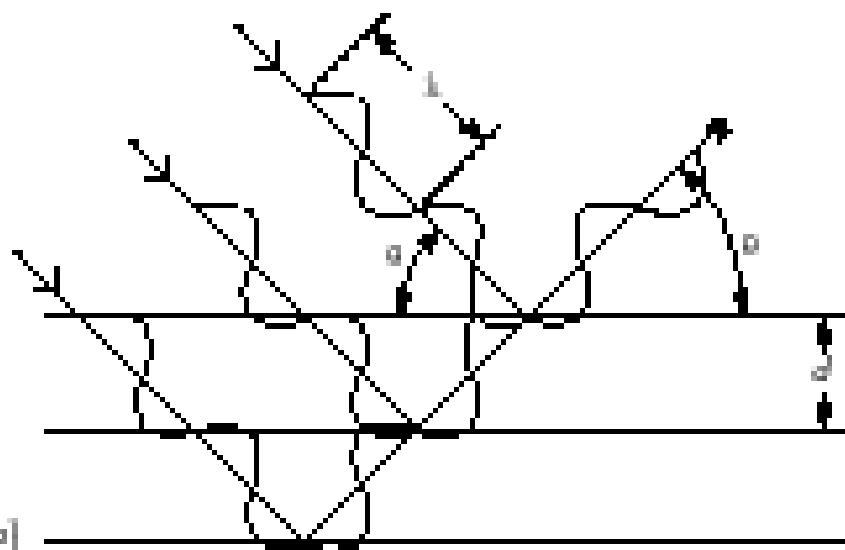
$$n \lambda = 2 d \sin \theta$$

and Bragg's Law has been derived. The location of the surface does not change the derivation of Bragg's Law.

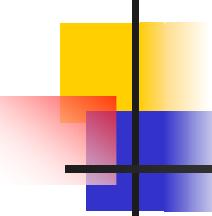
# Typical x-ray diffraction



Planes of high atomic density



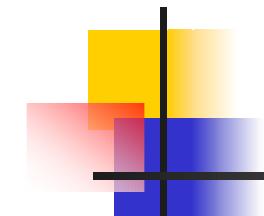
Scatter and diffraction from an ordered arrangement of atoms. (Reproduced from Jenkins, *X-ray Fluorescence Spectrometry*, 2nd edition, Wiley-Interscience, 1999. With permission from John Wiley & Sons.)



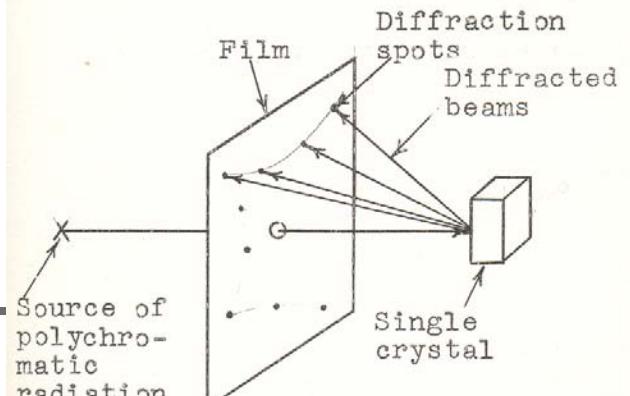
# APPLICATIONS



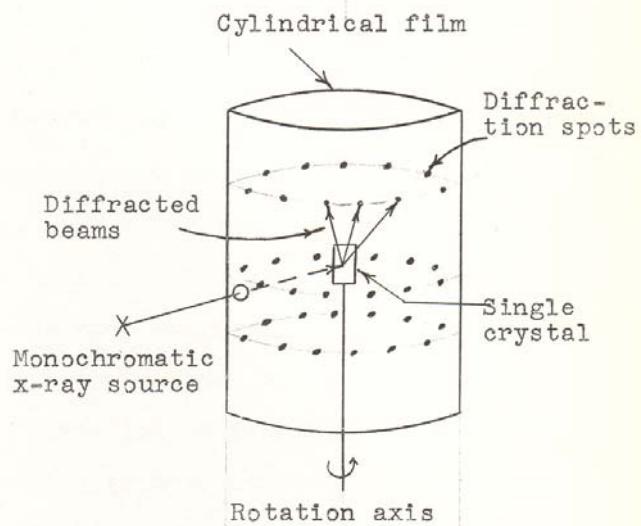
- **Identification** : The most common use of powder (polycrystalline) diffraction is chemical analysis.
  - This can include phase identification (search/match), investigation of high/low temperature phases, solid solutions and determinations of unit cell parameters of new materials.
- **Polymer crystallinity** : A polymer can be considered partly crystalline and partly amorphous.
  - The crystalline domains act as a reinforcing grid, like the iron framework in concrete, and improves the performance over a wide range of temperature.
  - However, too much crystallinity causes brittleness.
  - The crystallinity parts give sharp narrow diffraction peaks and the amorphous component gives a very broad peak (halo). The ratio between these intensities can be used to calculate the amount of crystallinity in the material.



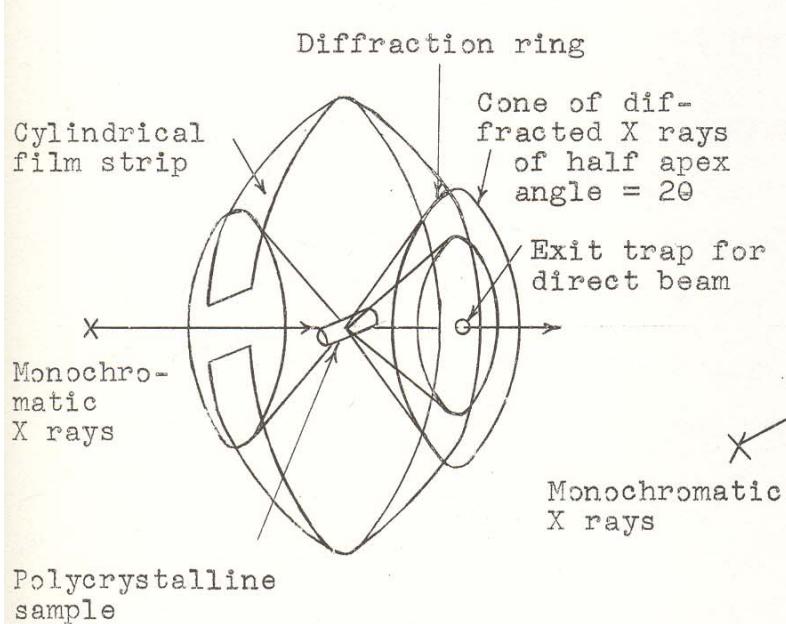
# Schematic Views of some X-Ray Diffraction Techniques



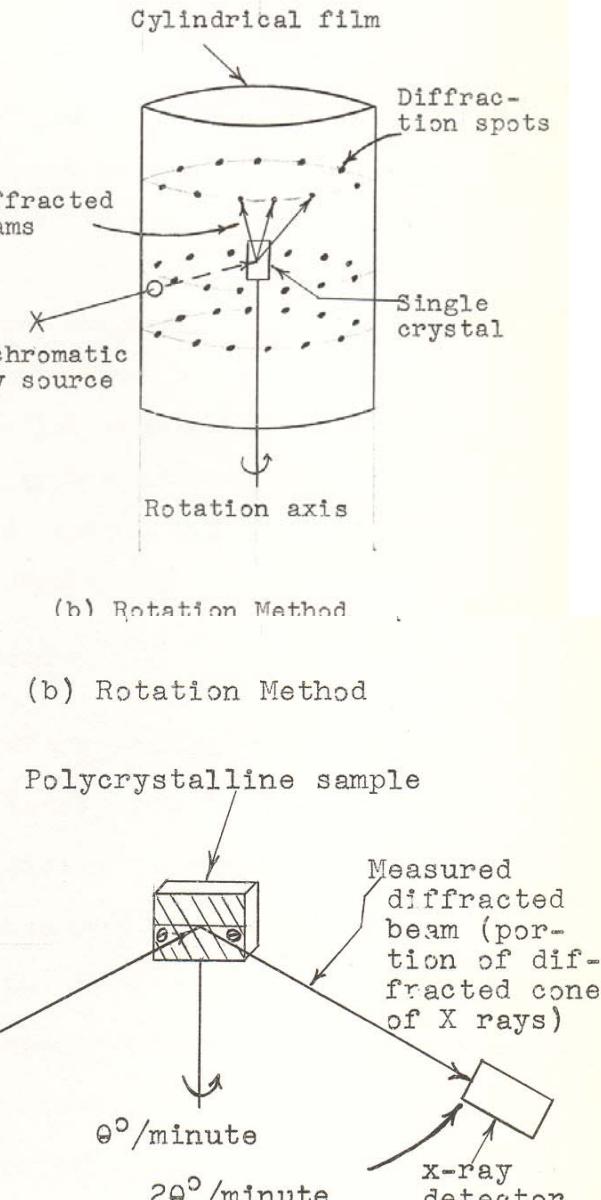
(a) Back-Reflection Laue Method



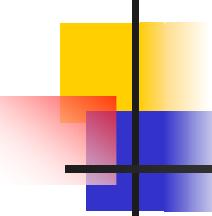
(b) Rotation Method



(c) Debye-Scherrer Method



(d) Diffractometer-powder Method



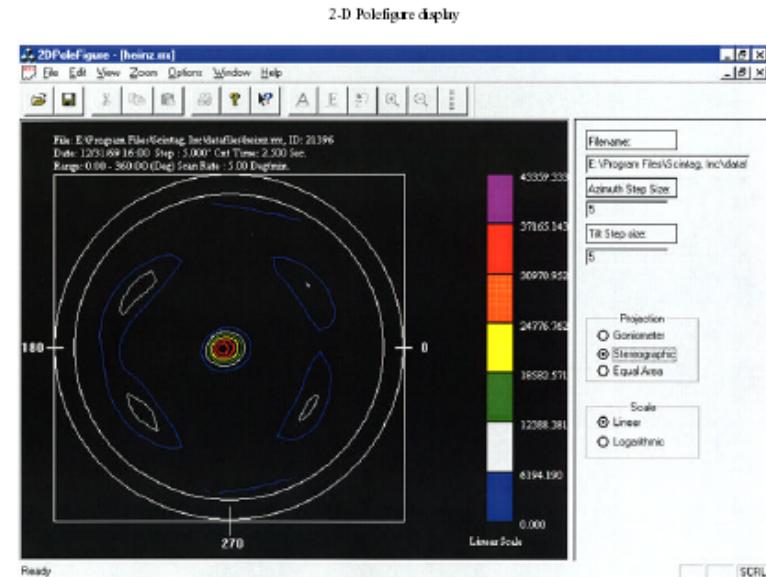
# Applications (cont'd)

- **Residual stress** : Residual stress is the stress that remains in the material after the external force that caused the stress have been removed.
  - Stress is defined as force per unit area. Positive values indicate tensile (expansion) stress, negative values indicate a compressive state.
  - The deformation per unit length is called strain.
- The residual stress can be introduced by any mechanical, chemical or thermal process. E.g. machining, plating and welding.
- The principals of stress analysis by the X-ray diffraction is based on measuring angular lattice strain distributions.
  - That is, we choose a reflection at high 2-Theta and measure the change in the d-spacing with different orientations of the sample.
  - Using Hooke's law the stress can be calculated from the strain distribution.

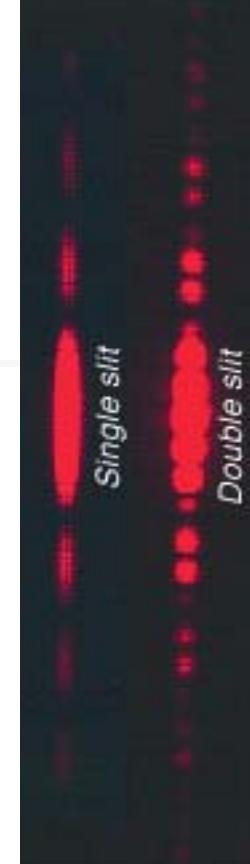
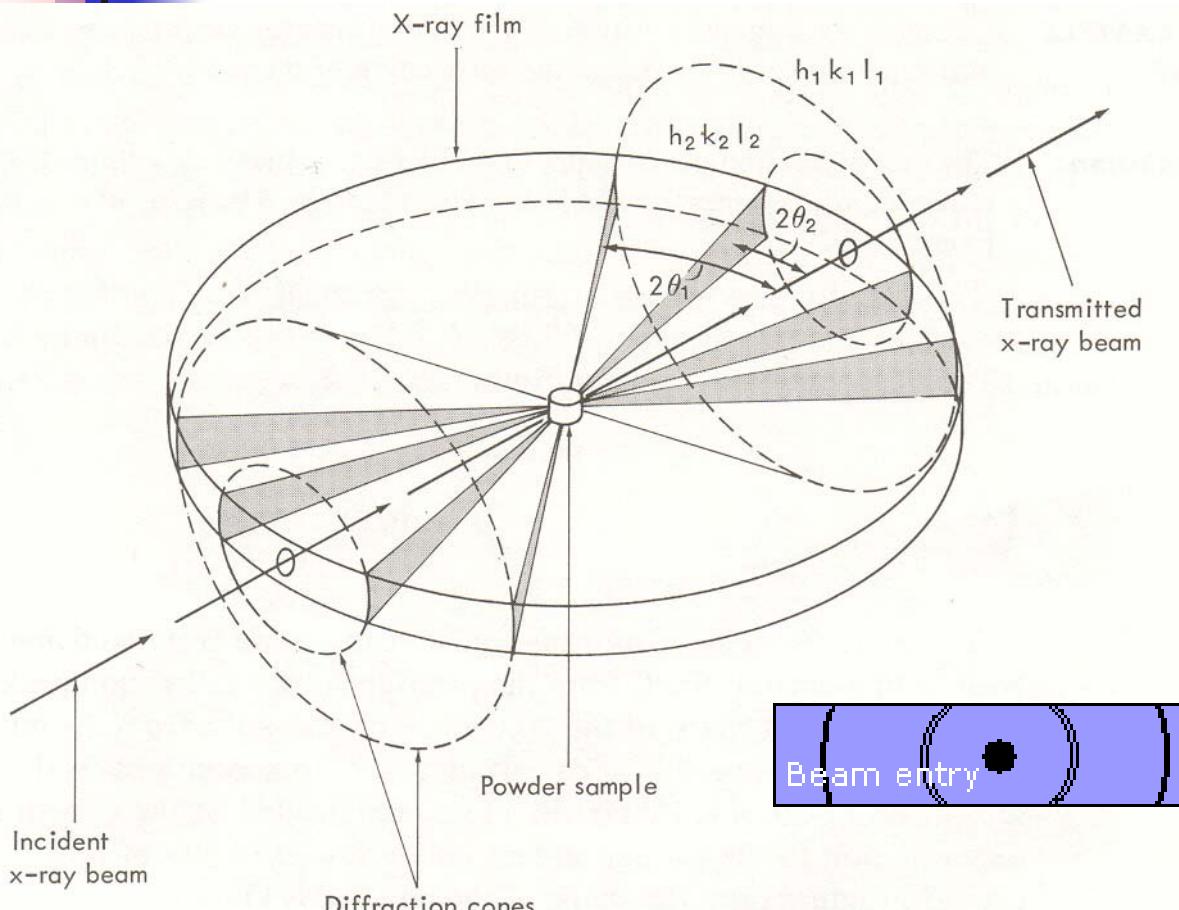
# Applications (cont'd)

- **Texture analysis** : The determination of the preferred orientation of the crystallites in polycrystalline aggregates is referred to as texture analysis, and the term texture is used as a broad synonym for preferred crystallographic orientation in the polycrystalline material, normally a single phase.

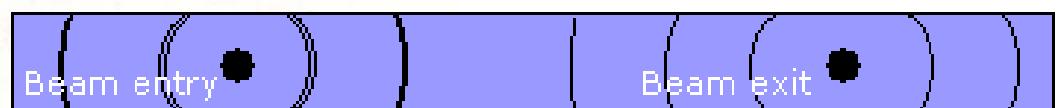
- The preferred orientation is usually described in terms of polefigures.
- A polefigure is scanned by measuring the diffraction intensity of a given reflection (2-Theta is constant) at a large number of different angular orientations of the sample.
- A contour map of the intensity is then plotted as a function of angular orientation of the specimen. The most common representation of the polefigures are stereographic or equal area projections. The intensity of a given reflection ( $h, k, l$ ) is proportional to the number of  $h, k, l$  planes in reflecting condition (Bragg's law).
- Hence, the polefigure gives the probability of finding a given crystal-plane-normal as function of the specimen orientation. If the crystallites in the sample have a random orientation the recorded intensity will be uniform.



# Powder x-ray diffraction

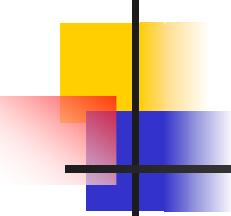


OD  
He-Ne Laser



XRD

Schematic illustration of the powder method. A strip of film surrounds the sample to record different diffraction peaks.



# Example 1

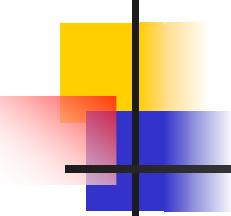
- Calculate the angular position of the first diffraction peak (lowest  $\theta$ ) for CsCl if the lattice parameter is 4.1 Å and the wavelength of the X-rays is 1.54 Å. The value of  $d_{100}$  is given by

$$d_{100} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} = \frac{4.1}{\sqrt{1}} = 4.1 \text{ \AA}$$

- The corresponding value of  $\theta$  is given by

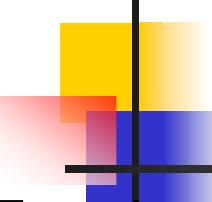
$$\sin \theta = \frac{\lambda}{2d} = \frac{1.54}{8.2} = 0.188$$

$$\theta = 10.3^\circ$$



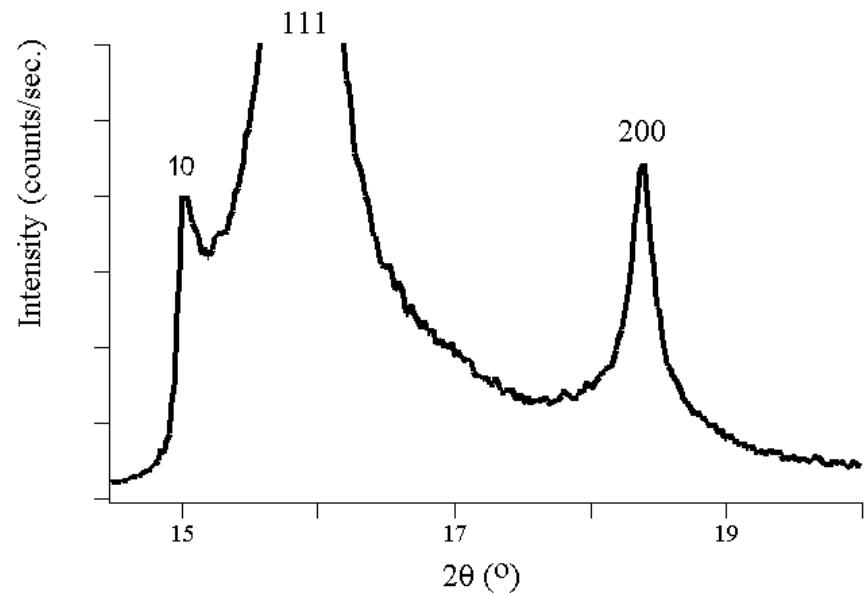
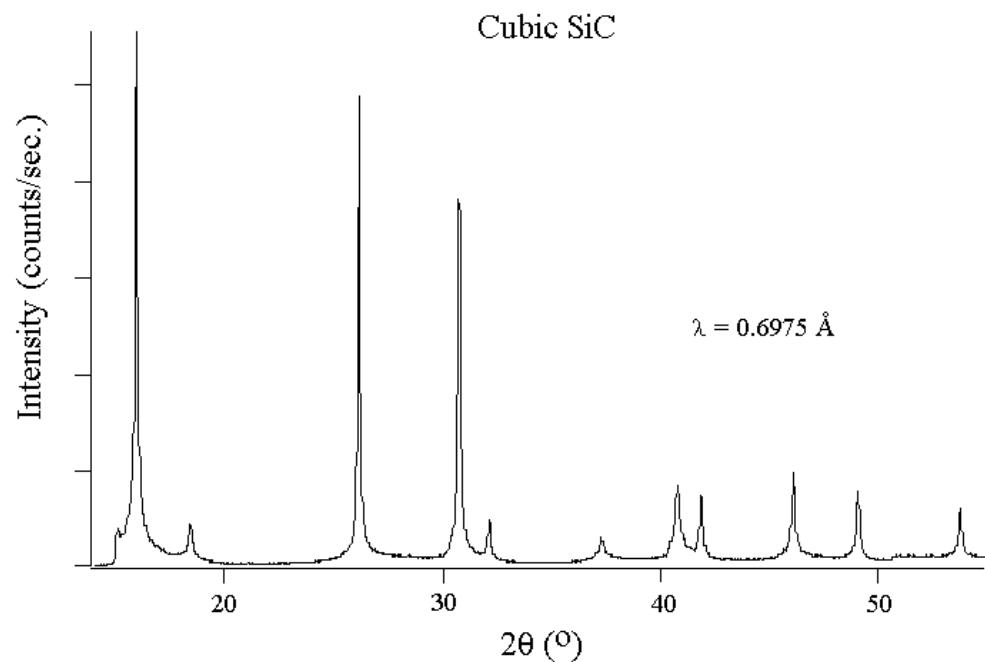
## Example 2

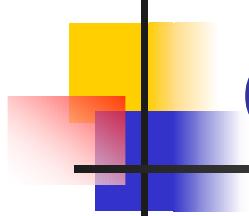
- The element Q belongs to the cubic crystal system.: From X-ray measurements it is known that the seven lowest order diffraction peaks occur at
  - $\sin^2 \theta = 0.137, 0.275, 0.412, 0.551, 0.688, 0.826, 0.962,$
  - What is the Bravais lattice?
- The  $\sin^2 \theta$  values are in the ratio 1, 2, 3, 4, 5, 6, 7. For the three cubic Bravais lattices the lowest order,  $1/d_{hkl}$  .and corresponding  $\sin^2 \theta$  values are in the ratios of  $(h^2 + k^2 + l^2)$  . We can evaluate the ratio of the allowed  $(h^2 + k^2 + l^2)$  values as:
  - Simple cubic 1, 2, 3, 4, 5, 6, 8, 9, 10
  - BCC 2, 4, 6, 8, 10, 12, 14, 16, 18
  - FCC 3, 4, 8, 11, 12, 16, 19
- The Bravais lattice of element Q is therefore BCC, since the observed  $\sin^2 \theta$  values are identical to the allowed  $(h^2 + k^2 + l^2)$  values.



# Experimental Diffraction Patterns

Experimental x-ray diffraction patterns of cubic SiC using synchrotron ( $\gamma$ ) radiation ( $\lambda = 0.6975 \text{ \AA} = 0.06975 \text{ nm}$ )





# Rules governing the presence of diffraction peaks

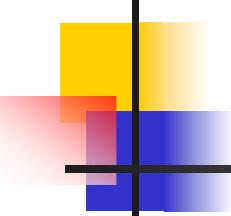
Bravais Lattice	Reflections Present	Reflections Absent
Simple Cubic	All	None
Body Centered Cubic	$(h+k+l)=\text{even}$	$(h+k+l)=\text{odd}$
Face Centered Cubic	$h,k,l$ unmixed*	$h,k,l$ mixed

\*  $h,k,l$  are either all odd or all even

# Peaks (reflection)for cubic lattices

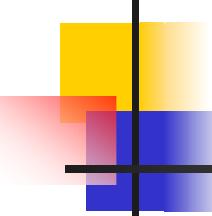
Table A4.1 Occurrence of reflections for the cubic crystal structures

Line no. $N =$ $h^2 + k^2 + l^2$	hkl indices	$N^{1/2} =$ $(h^2 + k^2 + l^2)^{1/2}$	f.c.c. diamond	Line no. $N =$ $h^2 + k^2 + l^2$	hkl indices	$N^{1/2} =$ $(h^2 + k^2 + l^2)^{1/2}$	b.c.c. f.c.c. diamond
1	100	1.00		33	522, 441	5.745	
2	110	1.414	x	34	530, 433	5.831	x
3	111	1.732		x	x	5.916	x x
4	200	2.00	x	x	x	6.00	x x x
5	210	2.236		36	600, 442	6.083	
6	211	2.450	x	37	610	6.164	
7	—	—		38	611, 532	6.325	
8	220	2.828	x	x	x	6.403	x x x
9	300, 221	3.00		40	620	6.481	
10	310	3.162	x		41	621, 540, 443	6.557
11	311	3.317		x	x	6.633	x x x
12	222	3.464	x	x	43	630, 542	6.708
13	320	3.606		44	631	6.782	
14	321	3.742	x		45	700, 632	
15	—	—		46	710, 550, 543	7.00	
16	400	4.00	x	x	x	7.071	
17	410, 322	4.123		47	711, 551	7.141	
18	411, 330	4.243	x		50	720, 641	7.211
19	331	4.359		x	x	7.280	
20	420	4.472	x	x	52	721, 633, 552	7.349
21	421	4.583		53	640		
22	332	4.690	x		54	731, 553	
23	—	—		55	—	7.483	
24	422	4.899	x	x	x	7.550	
25	500, 430	5.00		56	722, 544	7.616	
26	510, 431	5.099	x		57	730	
27	511, 333	5.196		x	x	7.681	
28	—	—		58	731, 553		
29	520, 432	5.385		59	800	7.810	
30	521	5.477	x		60	732, 651	7.874
31	—	—		61	—		
32	440	5.657	x	x	x	8.00	x x x



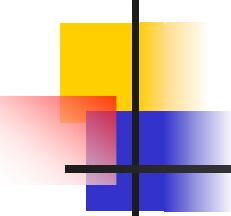
# Diamonds

- If we use X-rays with a wavelength ( $\lambda$ ) of  $1.54\text{\AA}$ , and we have diamonds in the material we are testing, we will find peaks on our X-ray pattern at  $\theta$  values that correspond to each of the d-spacings that characterize diamond.
- These d-spacings are  $1.075\text{\AA}$ ,  $1.261\text{\AA}$ , and  $2.06\text{\AA}$ . To discover where to expect peaks if diamond is present, you can set  $\lambda$  to  $1.54\text{\AA}$ , and set distance to one of the d-spacings.
- Then start with  $\theta$  at 6 degrees, and vary it until you find a Bragg's condition. Do the same with each of the remaining d-spacings. Remember that in the equations, you are varying  $\theta$ , while on the X-ray pattern printout, the angles are given as  $2\theta$ . Consequently, when the equations indicate a Bragg's condition at a particular angle, you must multiply that angle by 2 $\theta$  to locate the angle on the X-ray pattern printout where you would expect a peak.



# Symmetry operations

- Two objects are said to be **congruent** if to each point of one object corresponds a point of the other and if the distance between two points of an object is equal to the distance between corresponding points of the other.
- The corresponding angles will also be equal in absolute value. The congruence may be either **direct** or **opposite**, according to whether the corresponding angles have the same or opposite signs.
- For **direct** congruents, the objects can be superimposed, one object being brought to coincide with the other by a movement that may be :
  - - a **translation following a direction**
  - - a **rotation around an axis**
  - - a **rototranslation (screw movement)**, a combination of a translation and a rotation.



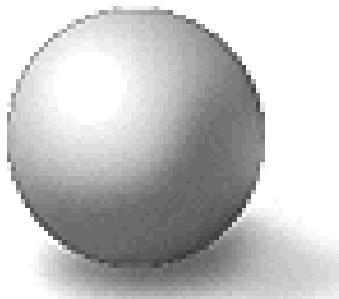
# Symmetry operations

- For **opposite** congruents, one object is said to be **enantiomorphous** with respect to the other (images in a mirror). The two objects may be brought to coincidence by the following operations :
  - - an **inversion** (versus a point)
  - - a **reflection** through a plane
  - - a **rotoinversion**, a combination of a rotation and an inversion
  - - a **reflection** combined with a **translation** parallel to the reflection plane (**glide** plane)
  - - a **rotoreflection**, a combination of a reflection and a rotation



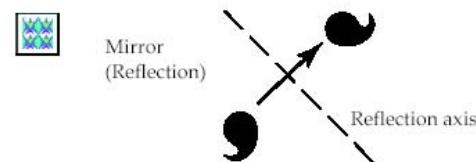
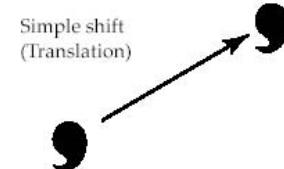
## Basic Symmetry Operations

**N-fold symmetry:**  
**The number of times**  
**one must rotate the**  
**object to make it**  
**coincident with the**  
**original.**

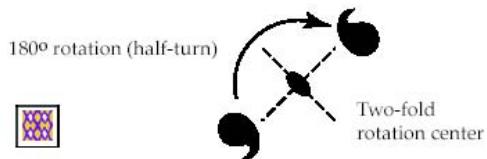
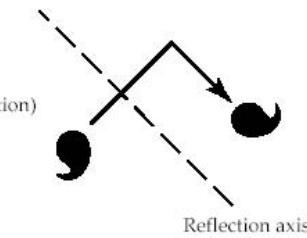


Sphere  
Infinite Symmetry

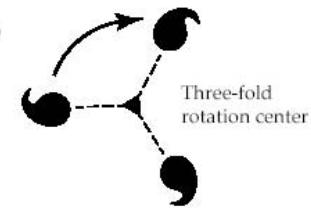
Is there a reflection? What is a glide-reflection? What other operations are used in the pattern design? There are only four basic operations that bring about an unending variety of symmetric patterns: translation, rotation, reflection, and glide-reflection. Here's the symmetry lingo at a glance. Use the symmetry types as indicated by SymmetryWorks icons to experiment with each symmetry operation.



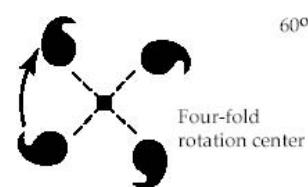
Glide-reflection  
(reflection + translation)



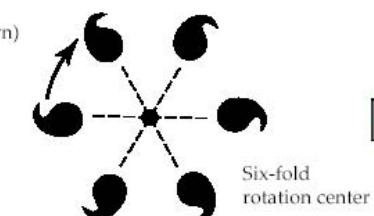
180° rotation (half-turn)



Three-fold  
rotation center

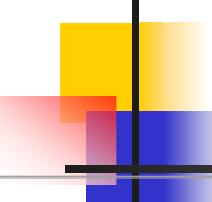


90° rotation (quarter-turn)

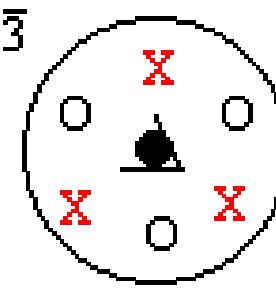
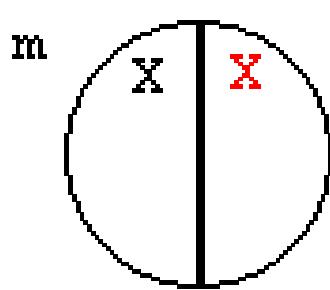
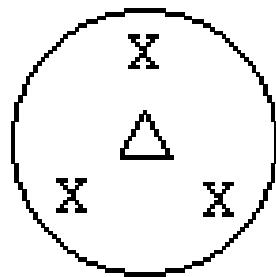
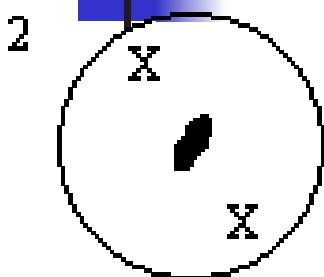


60° rotation (1/6-turn)

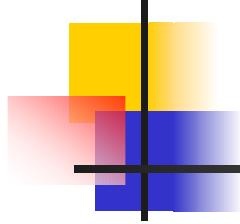




# Some symmetry elements

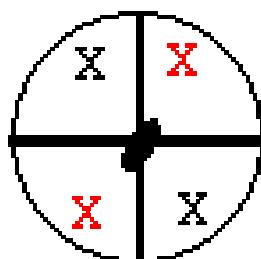


Some common symmetry elements (with their symbols) and their effect. x and o are used to represent the relative position of the objects (*e.g.* x = above the plane and o under the plane). For **opposite** congruents, a different color is given.

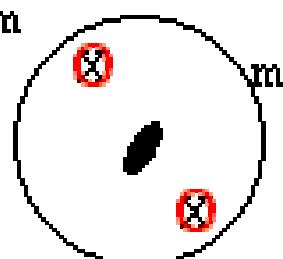


# Combination of symmetry elements

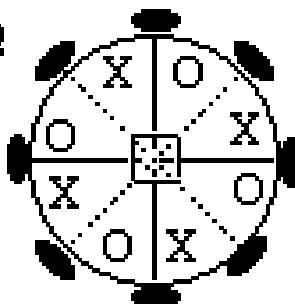
$2mm$



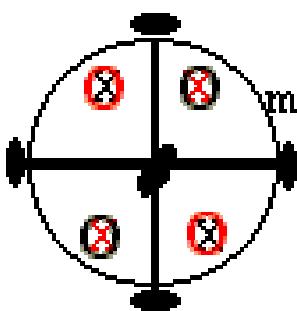
$2/m$



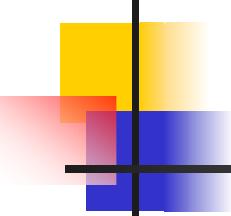
$422$



$2/mmm = mmmm$



Combination of symmetry elements. x and o are used to represent the relative position of the objects (*e.g.* x = above the plane and o under the plane). For **opposite congruents**, a different color is given.



# Point groups in 1D, 2D, or 3D objects

- The different combinations of symmetry elements that can be applied on finite 1D, 2D, or 3D objects are summarized in the Table.
- Note that planar molecules are usually considered as 2D objects.

1D		1 and -1					
2D	X	1	2	3	4	5	6
	Xm	m	2mm	3m	4mm	5m	6mm
3D	X	1	2	3	4	5	6
	-X	-1	-2 = m	-3 = 3-1	-4	-5 = 5-1	-6
	Xm	m	2mm	3m	4mm	5m	6mm
	X/m	m	2/m	3/m	4/m	5/m	6/m
	X2	2	222	32	422	52	622
	-Xm	-1m = 2/m	= 2mm	-3m	-42m	-5m	-62m
	X/mm	2mm	mmm	= -62m	4/mmm	5/mm	6/mmm
+ 7 groups		23, m3, 432, -43m, m3m, 532, -53m					