Theory of X-Ray Diffraction

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Introduction to X-Rays

- X-rays were discovered by the German Physicist Rontgen – he found that unlike ordinary light x-rays were invisible, but they traveled in straight lines and affected photographic film in the same way as light.

- X-rays are also more penetrating then light and could easily pass through the human body, wood, thick pieces of metal, and other opaque objects – an immediate application of this was the radiograph used by the physicians.

- In 1912 the exact nature of x-rays was established and in the same year the phenomenon of ***x-ray diffraction*** by crystals was discovered. This discovery provided a new method for investigating the fine structure of matter.

More Facts about X-Rays

- We now know that X-rays are electromagnetic radiation of exactly the same nature as light but of very shorter wavelength (10^{-10} m = 1 Angstrom). So X-rays are ideal to probe interatomic distances which are typically of that order.

- Typical energy scale = hc/λ = 12.3 KeV which is the characteristic energy of x-rays.

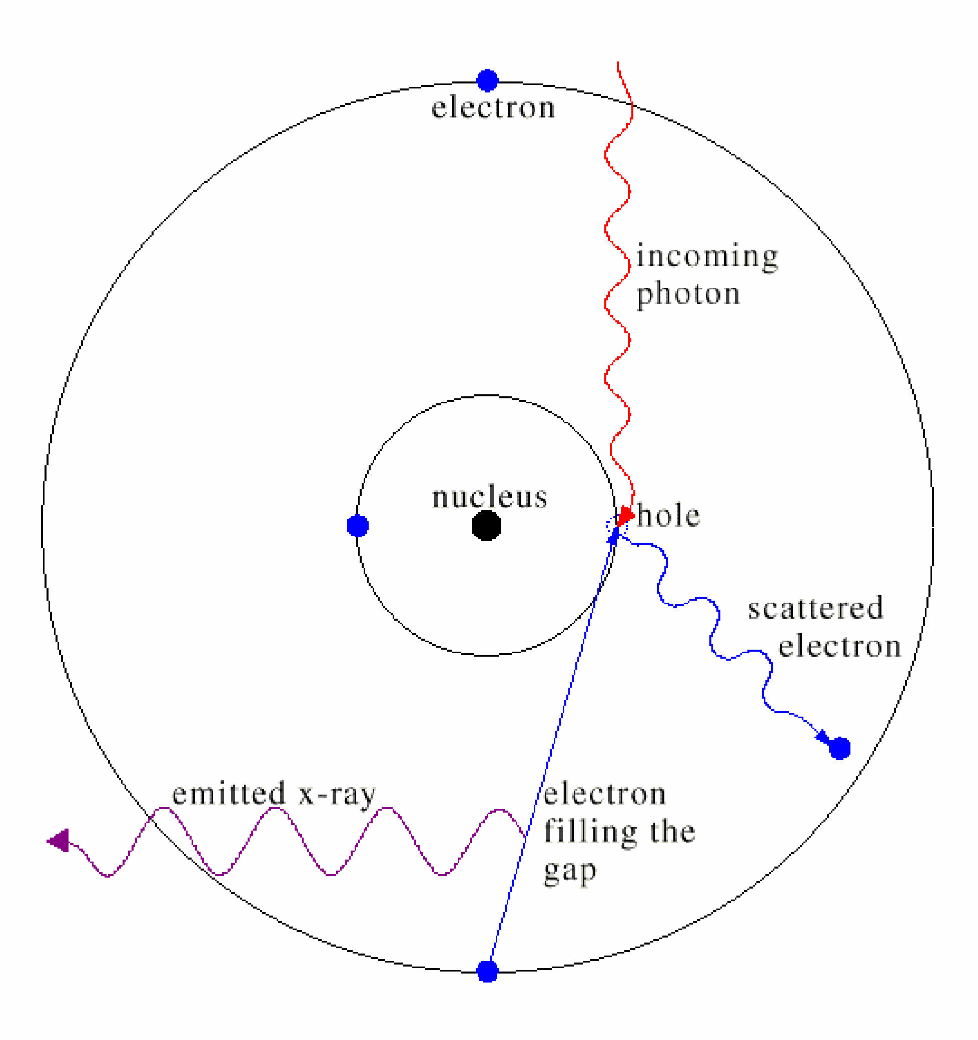
How do you get X-rays?

How does the X-ray spectrum look like?

X-rays are high-energy photons that are produced when electrons make transitions from one atomic orbit to another.

These transitions can be generated via the photoelectric effect as shown. If you send a photon into an atom with an energy greater than the binding energy of an electron in that atom, the photon can knock that electron out of its orbit, leaving a hole (or vacancy). This hole can then be filled by another electron in the atom, giving off an x-ray in the transition to conserve energy. This process is known as fluorescence.

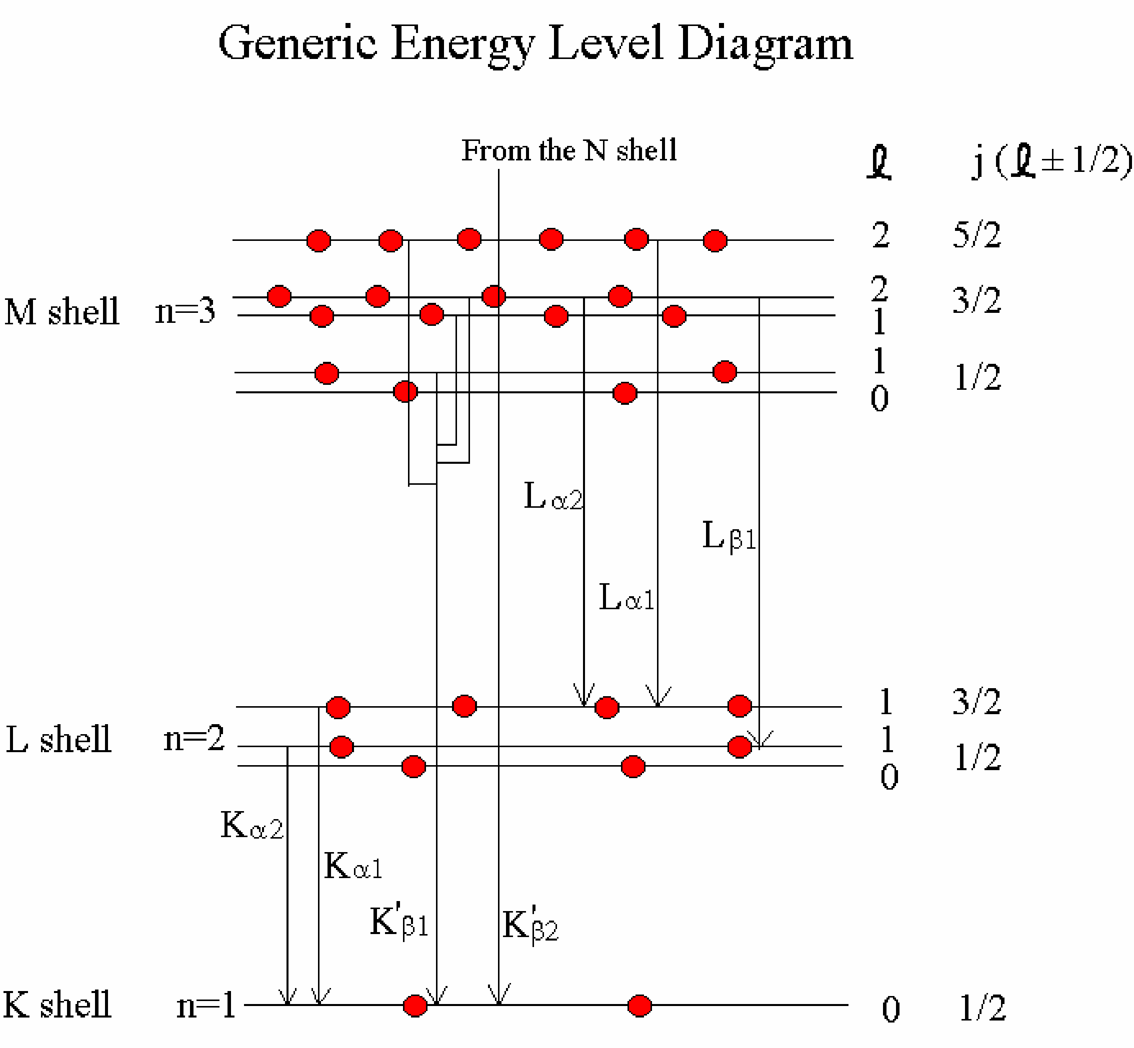
Many different atomic electrons of different binding energies can fill this hole, so you would expect to see many energy peaks in an x-ray spectrum.

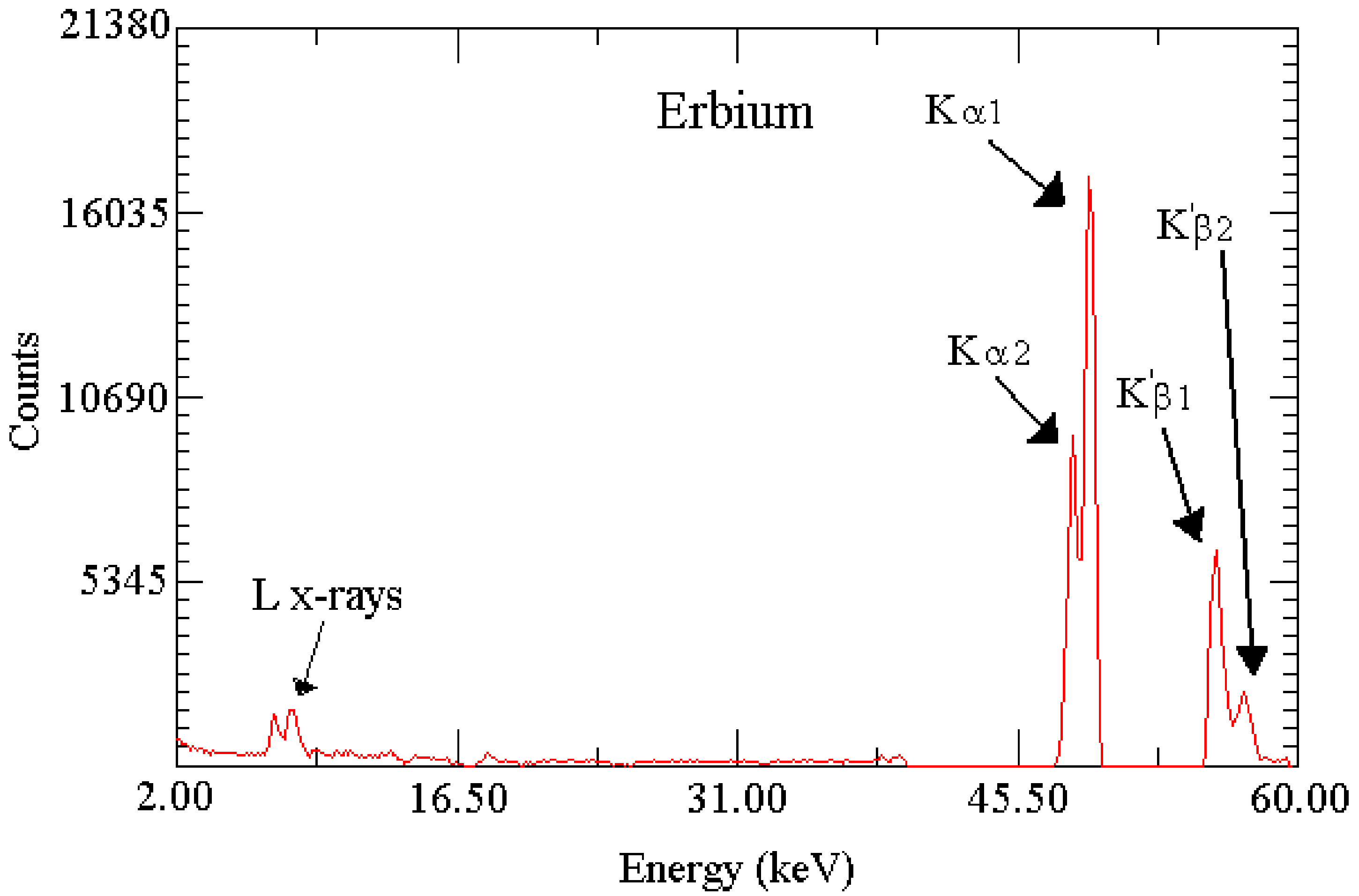


Electron transitions to the K shell of an atom are called K X-rays, and transitions to the L shell are called L X-rays. Not only are energy levels labeled, but specific atomic transitions are labeled also. Some of these labels are displayed in the Figure.

The $K_{\alpha1}$ x-ray is emitted in a transition from the n = 2, j = 3/2 level to the K-shell; the $K_{\alpha2}$ x-ray is emitted in a transition from the n = 2, j = 1/2 level to the K-shell.

The $K'_{\beta1}$ transition is a combination of all the transitions from the M shell to the K shell and the $K'_{\beta2}$ transition is a combination of all the transitions from the N shell to the K shell.



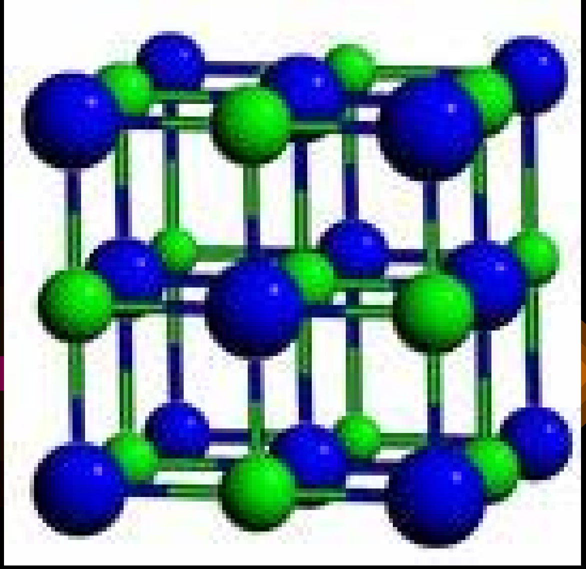


An X-ray spectrum of erbium (Z = 68) showing both K and L x-rays. Notice that the L x-rays have lower energy than the K x-rays due to the fact that the allowed electron levels of an atom get closer together in energy as n increases.

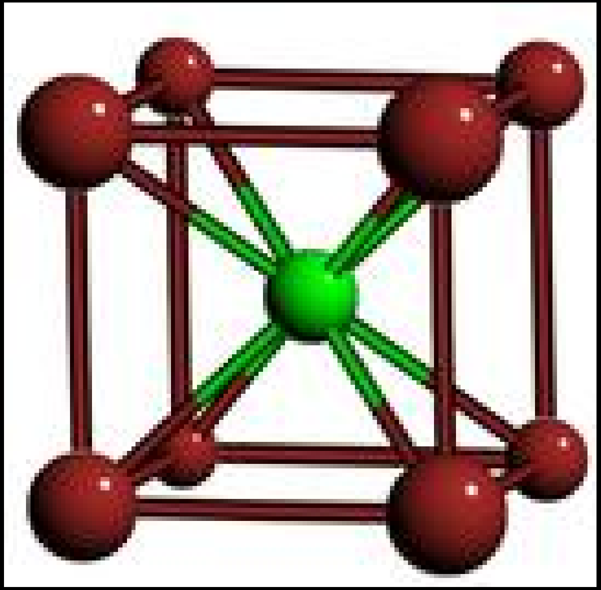
Crystal Structures

Lattices

- A crystal may be defined as a solid composed of atoms, ions or molecules arranged in a pattern periodic in three dimensions.
- Many solids are crystalline – single crystals or polycrystalline.
- Not all solids are crystalline, however; some are amorphous, like glass, and do not have any regular interior arrangement of atoms, ions, or molecules.
- Ignoring the actual atoms, ions, or molecules we will focus on the geometry of periodic arrays – the crystal is then represented as a lattice, i.e. a three dimensional array of points (lattice points) each of which has identical surroundings.



NaCl Structure



CsCl Structure

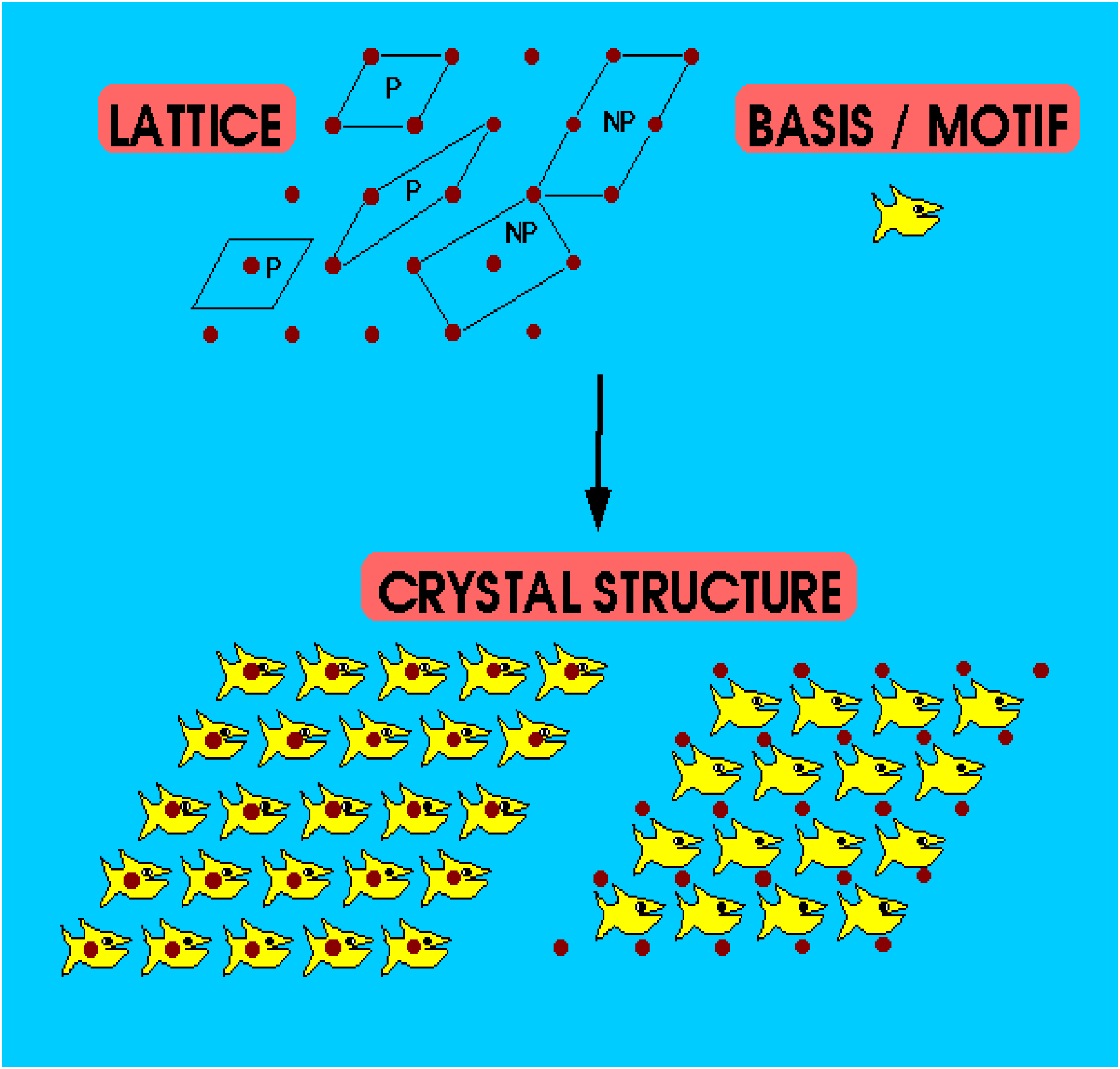
- Two distinct concepts in crystallography:

  Lattice: consists of points in geometrical arrays,

  Basis: describes the arrangement of atoms associated with each lattice point.

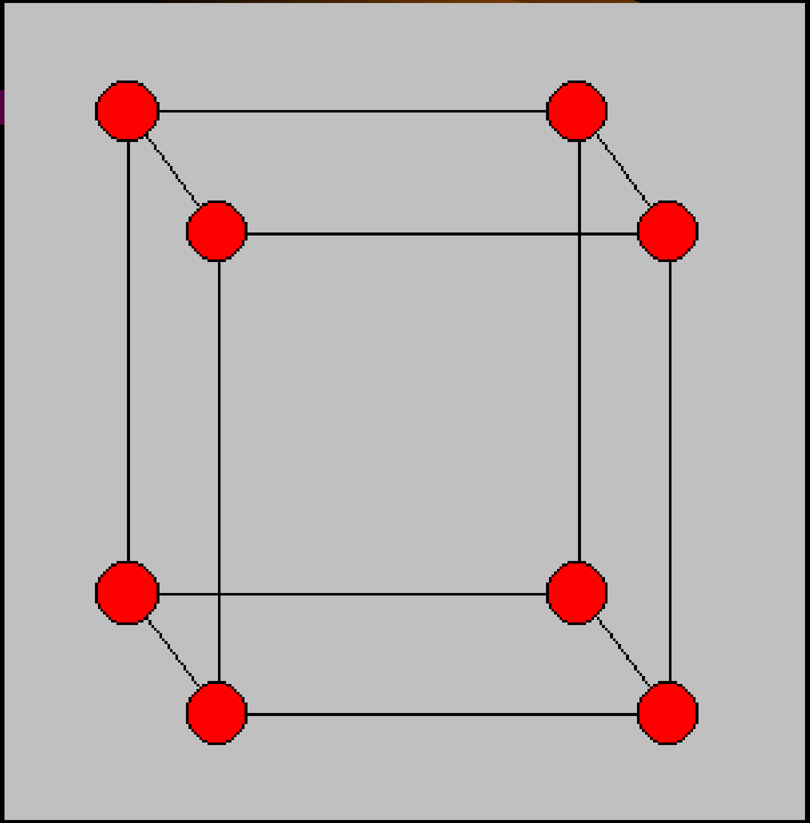
Crystal Structure

= Lattice + Basis



Bravais Lattice

(Two equivalent descriptions)

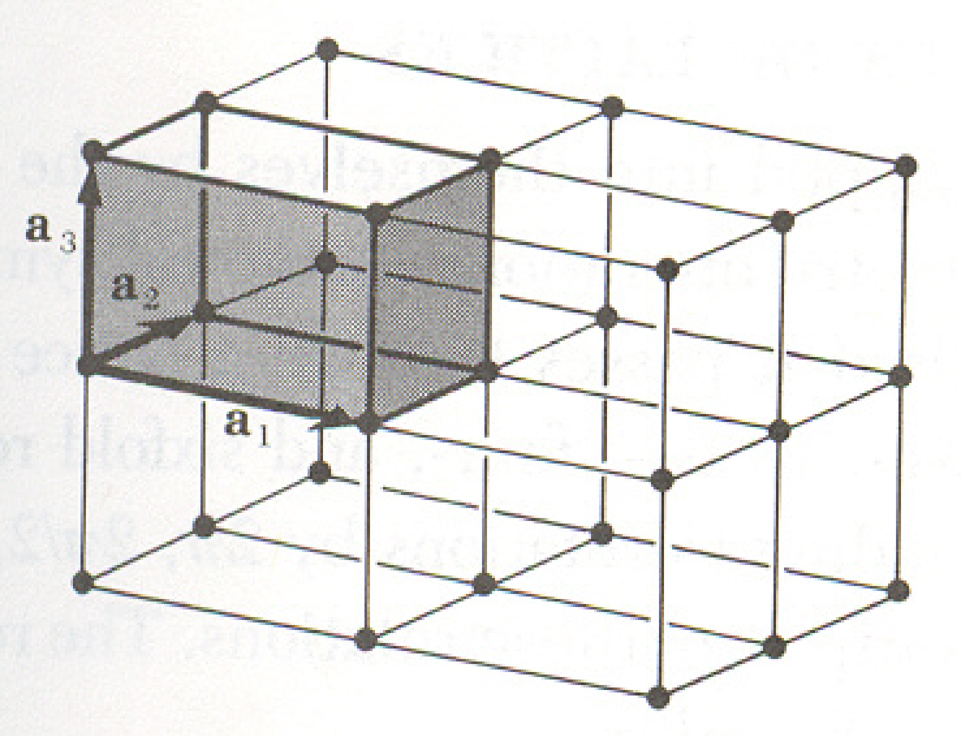


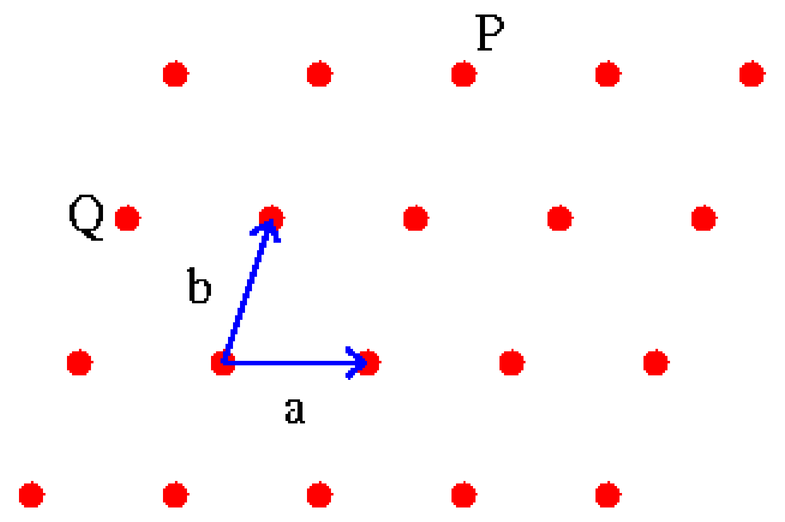
(a) It is an infinite array of discrete points with an arrangement and orientation that appears exactly the same, from whichever of the points the array is viewed.

(b) A 3D Bravais lattice consists of all points with position vectors **R** of the form $\mathbf{R} = p\,\mathbf{a} + q\,\mathbf{b} + r\,\mathbf{c}$, where p, q, r are integers and (**a,b,c**) are any 3 vectors.

Primitive vectors:

In 3D the vectors **(a, b, c)** define a unit cell of a Bravais lattice. These vectors are called primitive vectors and they are said to generate or span the lattice. Example of primitive vectors in a 3D Bravais lattice is shown below.





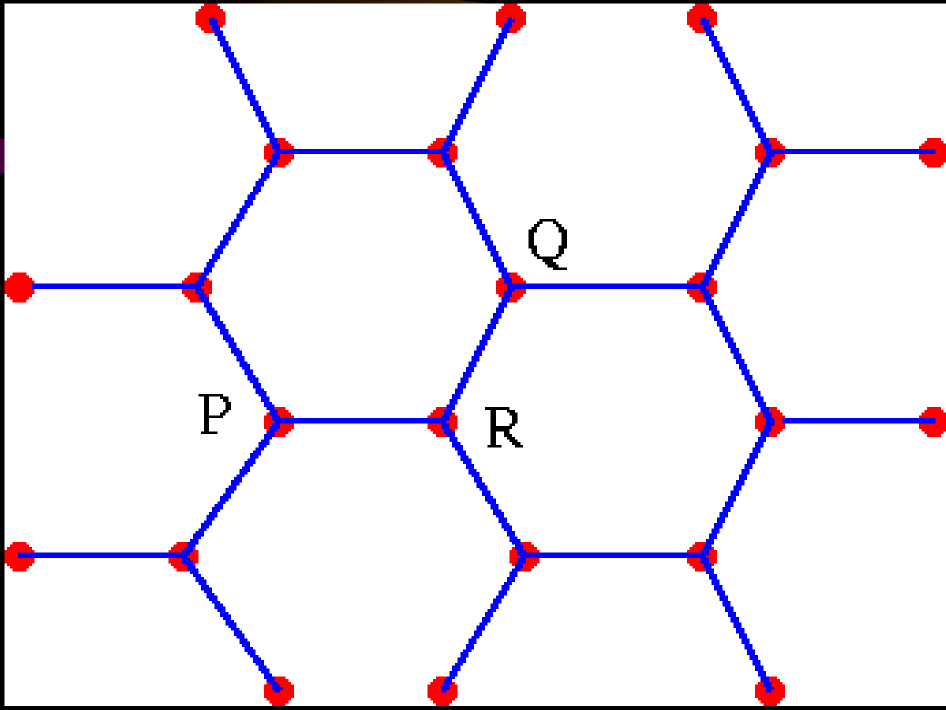
2D Bravais lattice of no particular symmetry: the oblique net. Primitive vectors are **(a, b).** All the points are linear combinations of these with integer coefficients for example: **P = a + 2b**, **Q = -a + b** etc.

Is this a Bravais lattice?

It’s not a Bravais lattice!

The arrays of points look the same whether viewed from points P or Q.

But the view from point R is rotated by 180°. So it’s not a Bravais lattice.



The vertices of a 2D honeycomb lattice.

Lesson:

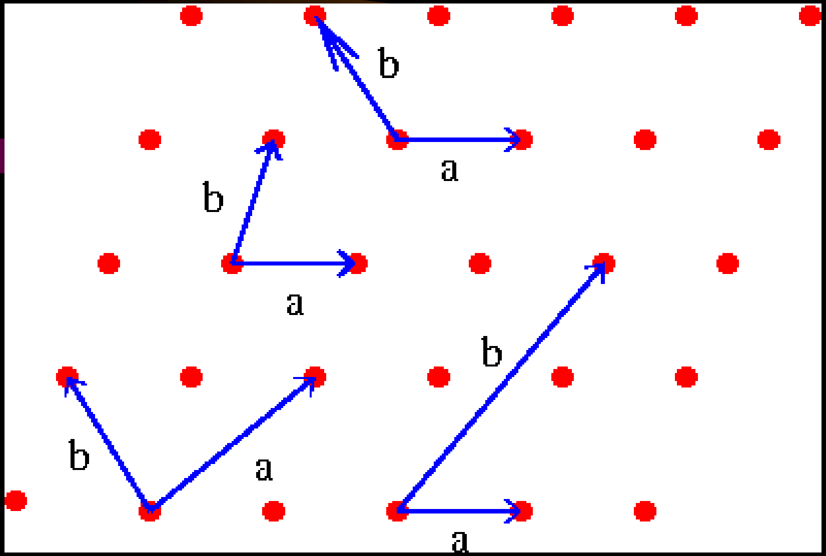
The arrangement and orientation both must appear the same from every point in a Bravais lattice.

Infinite Lattices and Finite crystals:

For a Bravais lattice since all points are equivalent it must be infinite in extent. (idealization)

But actual crystals are finite! If the crystals are large enough the vast majority of points will be so far from the surface that one can neglect the surface boundaries.

There are cases where surface effects are important – then the notion of Bravais lattice is still relevant, but then one must think of the physical crystal as filling up a finite portion of the ideal Bravais lattice.



Are the primitive vectors unique?

No! There are infinitely many nonequivalent choices!!

More examples

Simple Cubic Lattice (SC):

A choice of primitive vectors are the three orthogonal vectors

(a ***x***, a ***y***, a ***z***).

(Note: ***x***, ***y***, ***z*** are unit vectors)

Body Centered Cubic (BCC):

A set of primitive vectors are:

a = a ***x***,

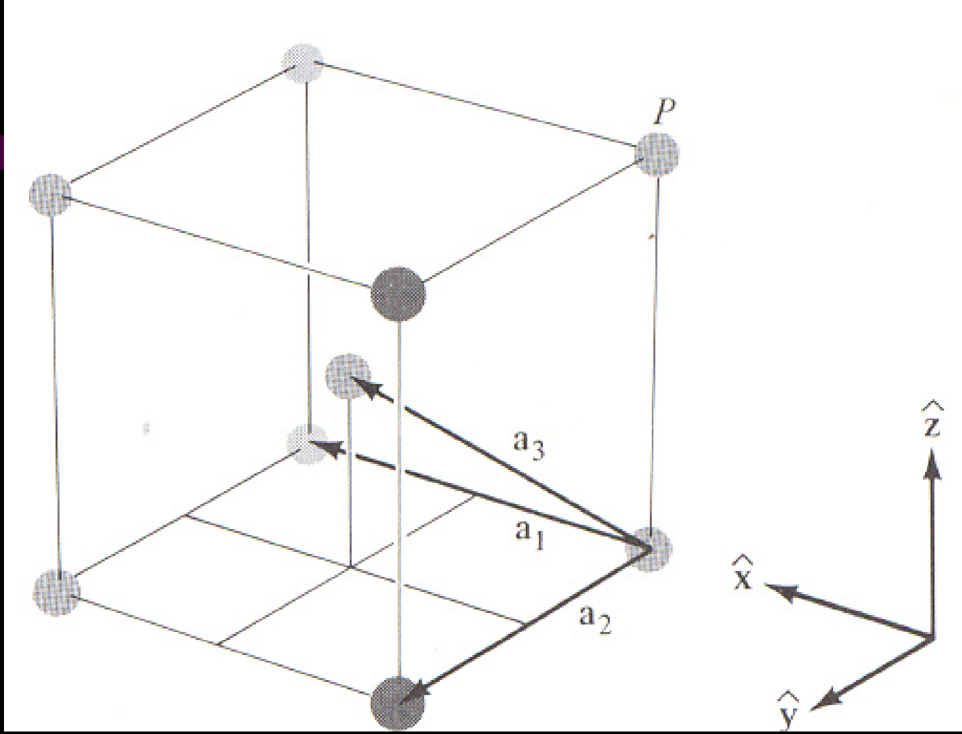
b = a ***y***,

c = a/2 (***x*** + ***y*** + ***z***).

Point P for example :

P = - **a** – **b** + 2**c**

(check that is is equal to a ***z***).

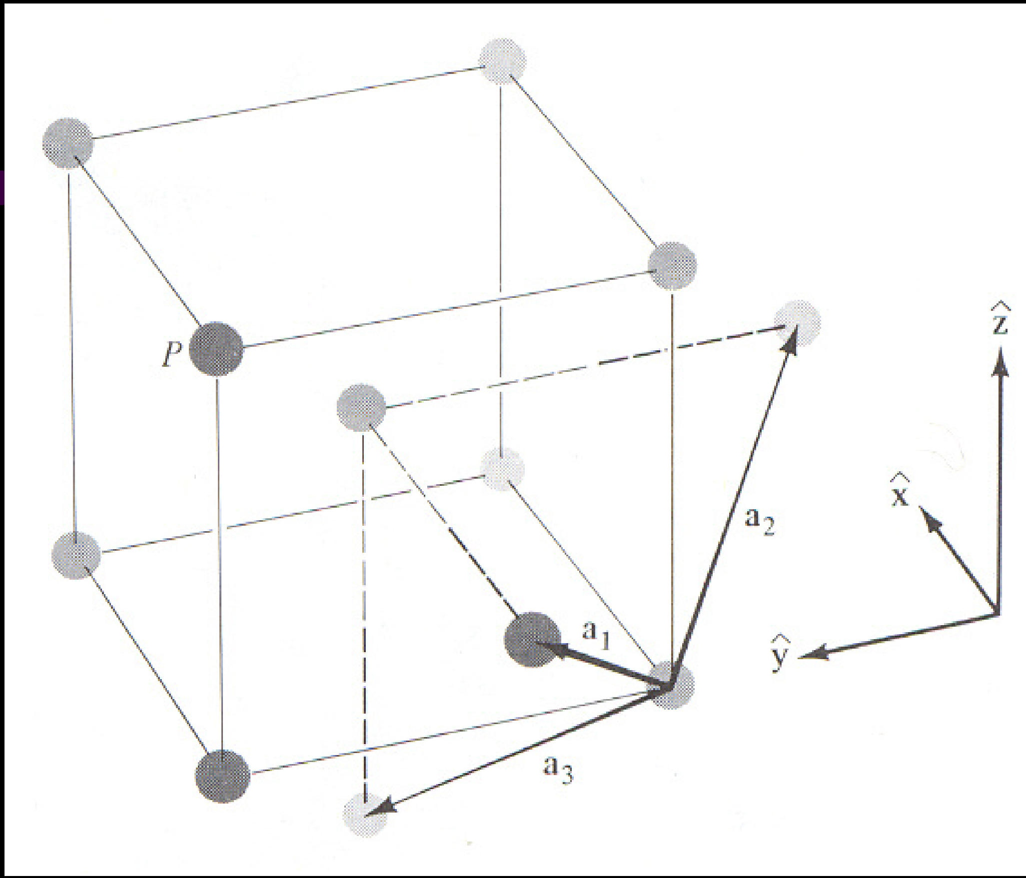


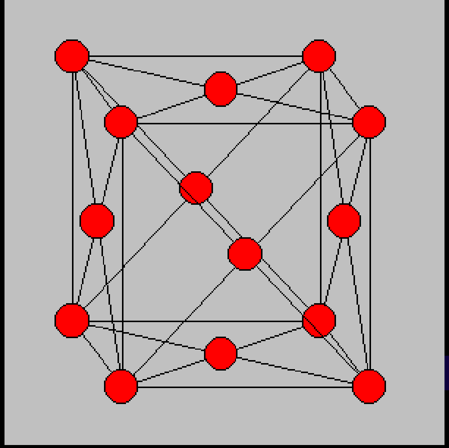
A more symmetric set of primitive vectors for the BCC lattice is

$\mathbf{a} = a/2\,(\boldsymbol{y} + \boldsymbol{z} - \boldsymbol{x})$,

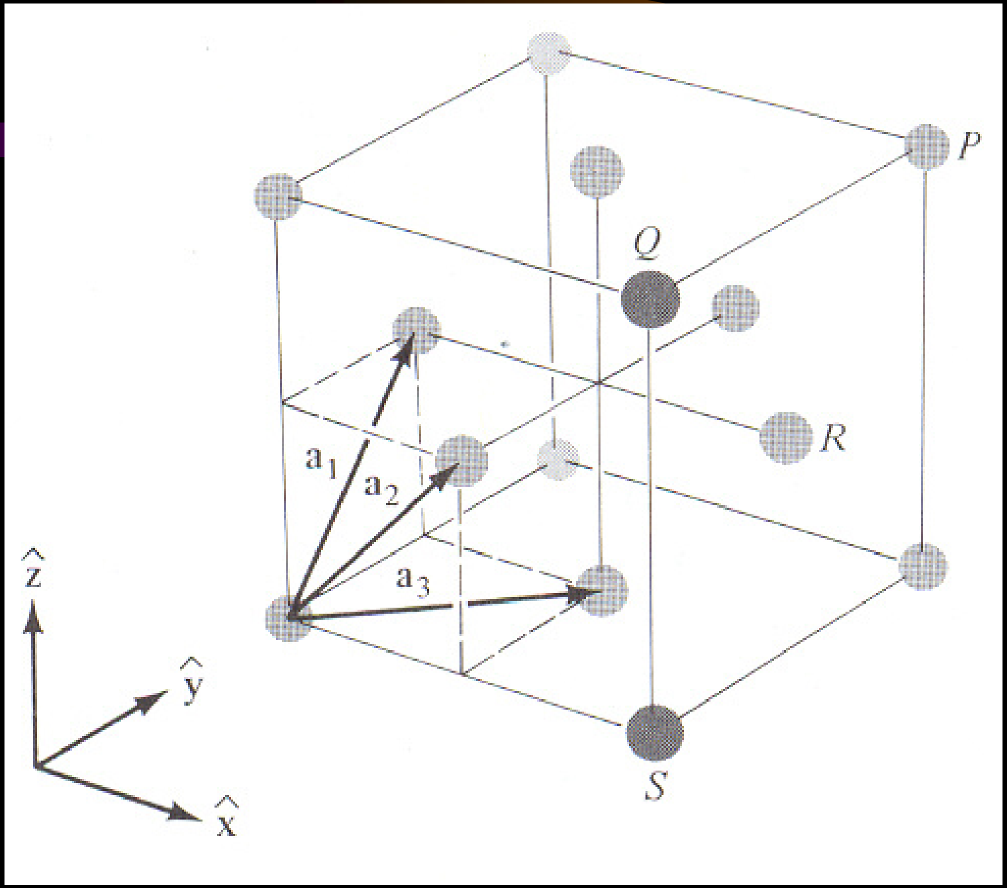
$\mathbf{b} = a/2\,(\boldsymbol{z} + \boldsymbol{x} - \boldsymbol{y})$,

$\mathbf{c} = a/2\,(\boldsymbol{x} + \boldsymbol{y} - \boldsymbol{z})$.





Face Centered Cubic (FCC) Lattice



A more symmetric set of primitive vectors for the BCC lattice is

$\mathbf{a} = a/2\ (y + z),$

$\mathbf{b} = a/2\ (z + x),$

$\mathbf{c} = a/2\ (x + y).$

$P = \mathbf{a} + \mathbf{b} + \mathbf{c}$, $Q = 2\mathbf{b}$,

$R = \mathbf{b} + \mathbf{c}$, $S = -\mathbf{a} + \mathbf{b} + \mathbf{c}$.

Coordination Number

The points in a Bravais lattice that are closest to a given point are called its ***nearest neighbors***.

Because of the periodic nature of the Bravais lattice, *each point has the same number of nearest neighbors*. ***This number*** is thus a property of the lattice, and is referred to as ***the coordination number of the lattice***.

Coordination numbers for

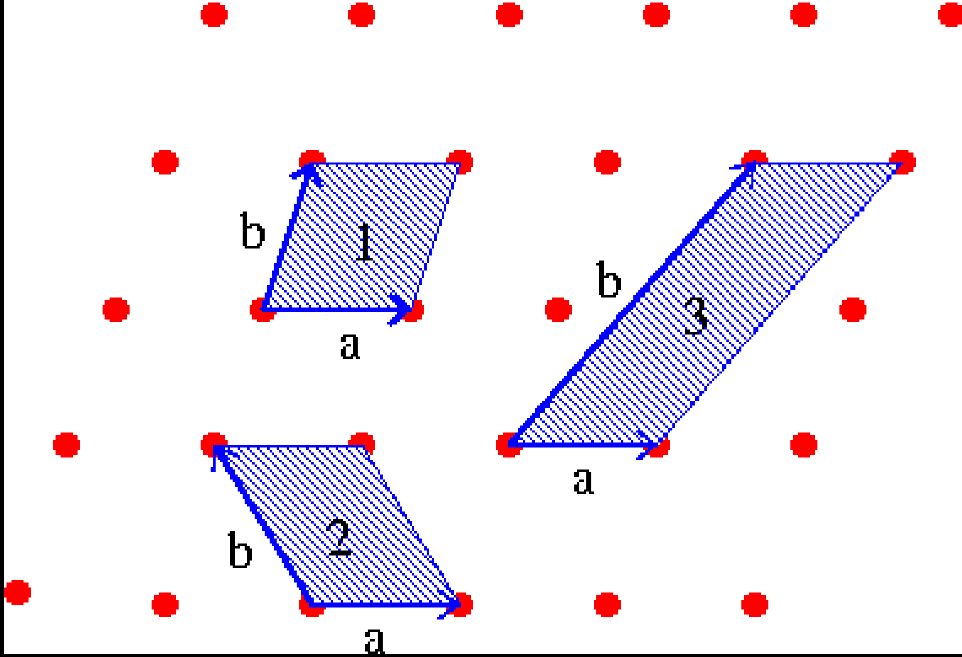
SC:	**6** (2 x 3)
BCC:	**8** (2 x 4)
FCC:	**12** (2 x 6)

Primitive Unit Cell

- The parallelepiped defined by the primitive vectors **(a, b, c)** is called a ***primitive cell*** or a ***unit cell***.

- A cell will fill all space by the repetition of suitable crystal translation operations.

- A primitive cell is a ***minimum volume cell*** and there are many ways of choosing the primitive axes and primitive cell for a given lattice.



Other Properties of Primitive Unit Cell

- The number of atoms in a primitive cell is always the same for a given lattice structure.

- There is always ***one lattice point per primitive cell***. If the primitive cell is a parallelepiped with lattice points at each of the 8 corners, each lattice point is shared among 8 cells, so that the total number of lattice points in the cell is one: 8 x (1/8) = 1.

- The volume of a parallelepiped with axes **(a, b, c)** is

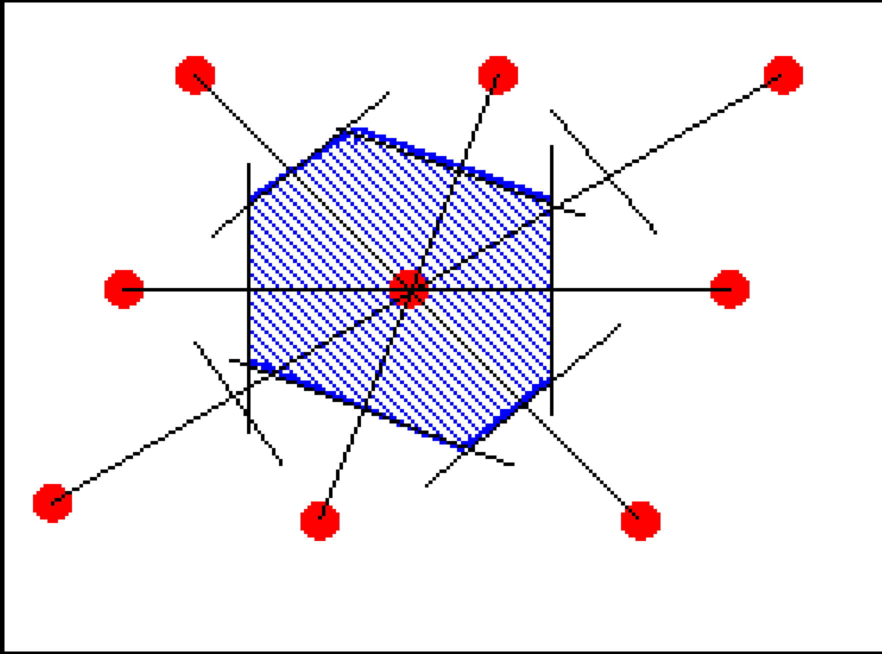
$$V_C = |\,\mathbf{a}\ .\ (\,\mathbf{b}\ \mathbf{x}\ \mathbf{c})\,|$$

Wigner-Seitz Primitive Cell

- Another way of choosing a ***primitive cell*** is known to physicists as a ***Wigner-Seitz cell***.

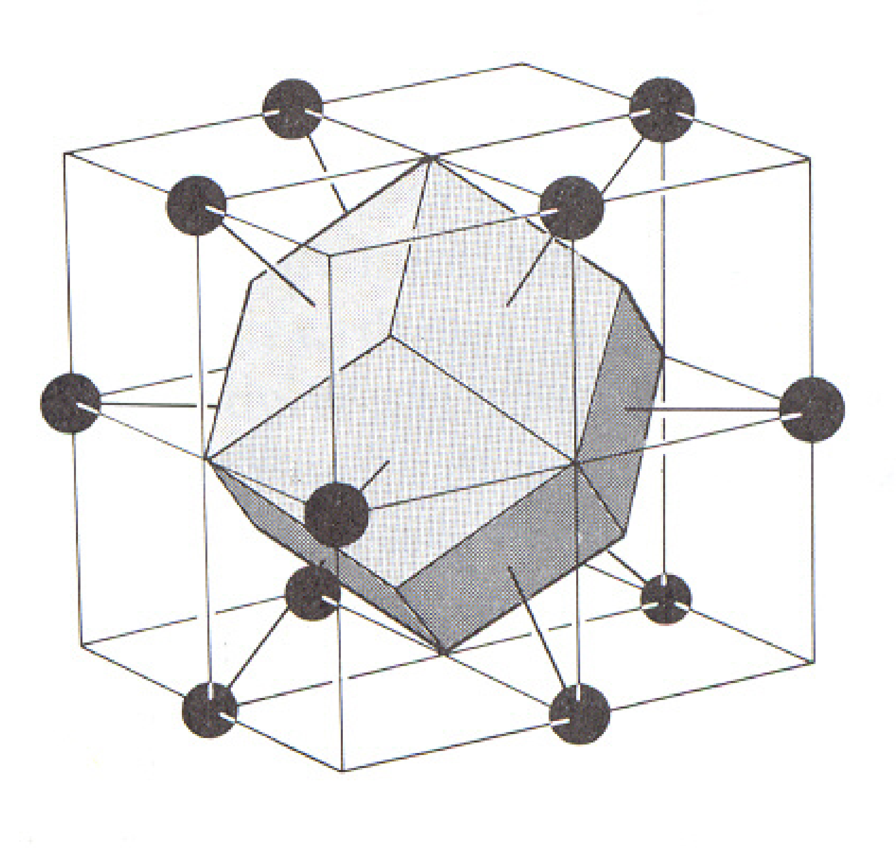
- **Wigner-Seitz cell for a 2D Bravais lattice:**

  The 6 sides of the cell bisect the lines joining the central points to its 6 neighboring points.

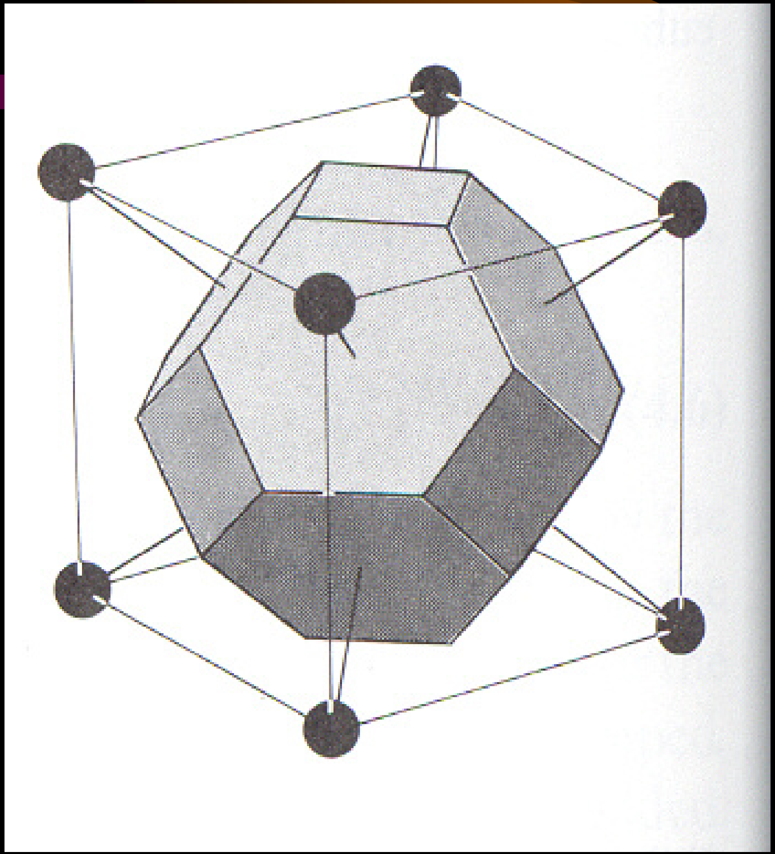


- In 2D, the Wigner-Seitz cell is always a hexagon unless the lattice is rectangular.

Wigner-Seitz Primitive Cell in 3D



Wigner-Seitz primitive cell for the BCC Bravais lattice
(a “truncated octahedron”)

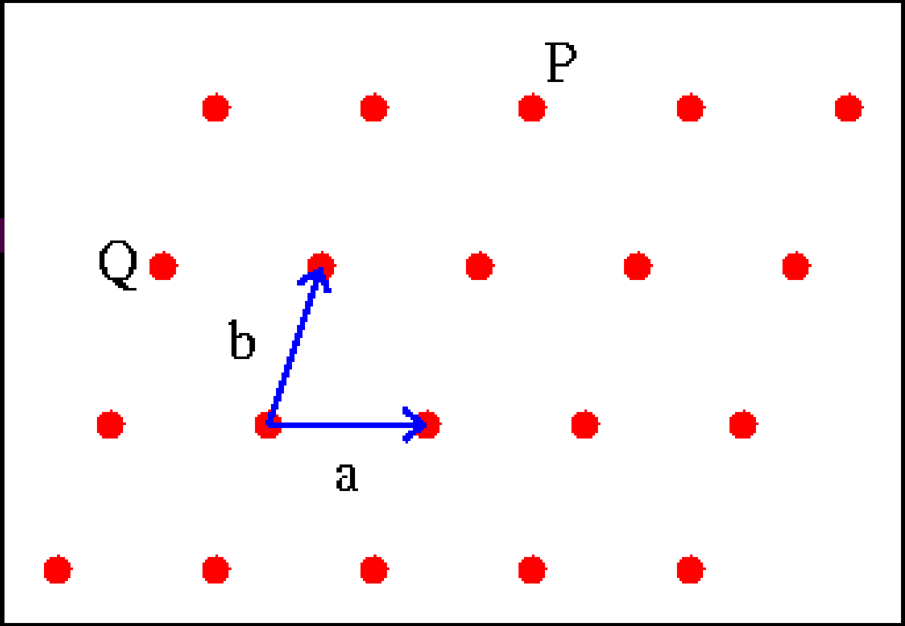


Wigner-Seitz primitive cell for theFCC Bravais lattice
(a “rhombic dodecahedron ”)

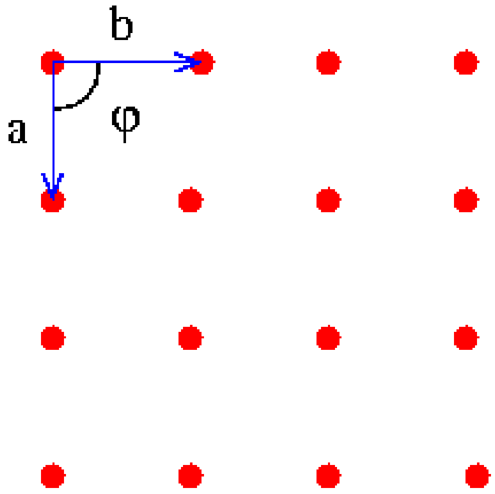
Fundamental Types of Lattices

2D Lattice Types

- In 2D there are infinite number of possibilities.
- A general lattice is the oblique lattice and is invariant only under rotation of π and 2π about any lattice point.
- There are 4 special lattice type: ***Square lattice, Rectangular lattice, Hexagonal lattice, and Centered rectangular lattice***.
- So, **there are 5 distinct types of lattices in 2D**.

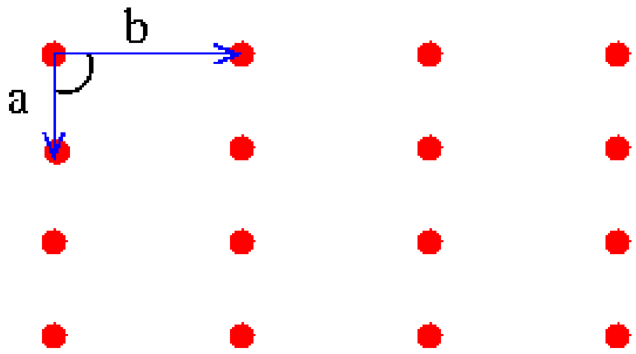


Oblique Lattice



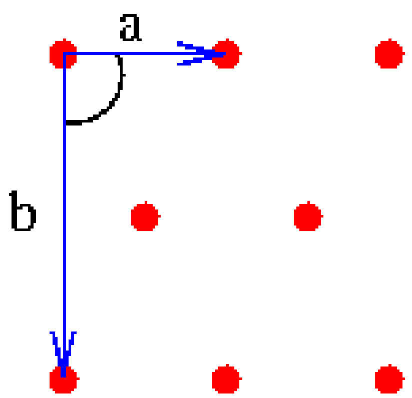
Square Lattice

$|a| = |b|; \quad \varphi = 90^\circ$



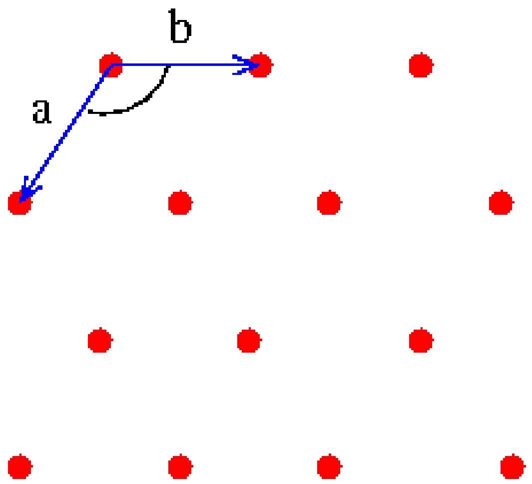
Rectangular Lattice

$|a| \neq |b|, \quad \varphi = 90^\circ$



Centered Rectangular Lattice

$\varphi = 90^\circ$



Hexagonal Lattice

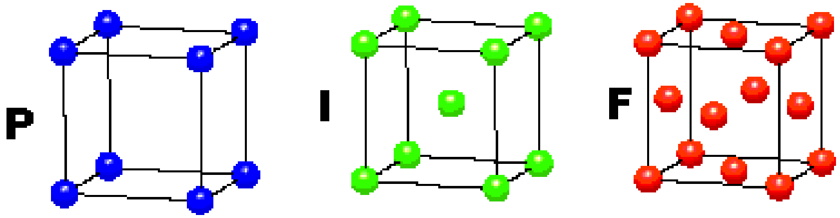
$|a| = |b|; \quad \varphi = 120^\circ$

3D Lattice Types

CUBIC

$a = b = c$

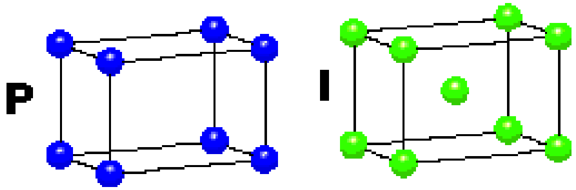
$\alpha = \beta = \gamma = 90°$



TETRAGONAL

$a = b \neq c$

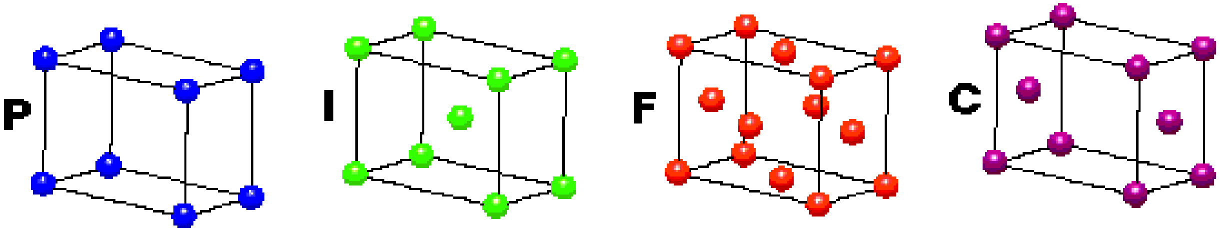
$\alpha = \beta = \gamma = 90°$



ORTHORHOMBIC

$a \neq b \neq c$

$\alpha = \beta = \gamma = 90°$

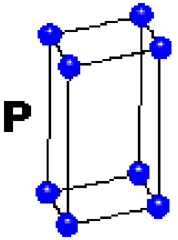


HEXAGONAL

$a = b \neq c$

$\alpha = \beta = 90°$

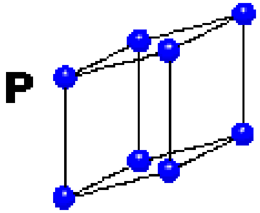
$\gamma = 120°$



TRIGONAL

$a = b = c$

$\alpha = \beta = \gamma \neq 90°$

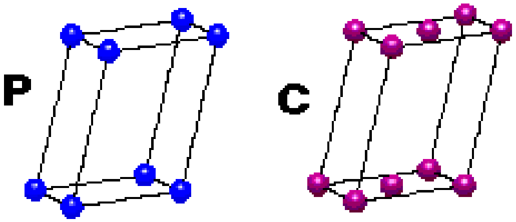


MONOCLINIC

$a \neq b \neq c$

$\alpha = \gamma = 90°$

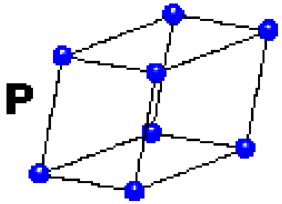
$\beta \neq 120°$



TRICLINIC

$a \neq b \neq c$

$\alpha \neq \beta \neq \gamma \neq 90°$



4 Types of Unit Cell
P = Primitive
I = Body-Centred
F = Face-Centred
C = Side-Centred
\+
7 Crystal Classes
→ 14 Bravais Lattices

Index system for Crystal planes

- It is a standard practice to describe directions in the crystal by a vector related to the principal axes of the system.

- A general vector of the form

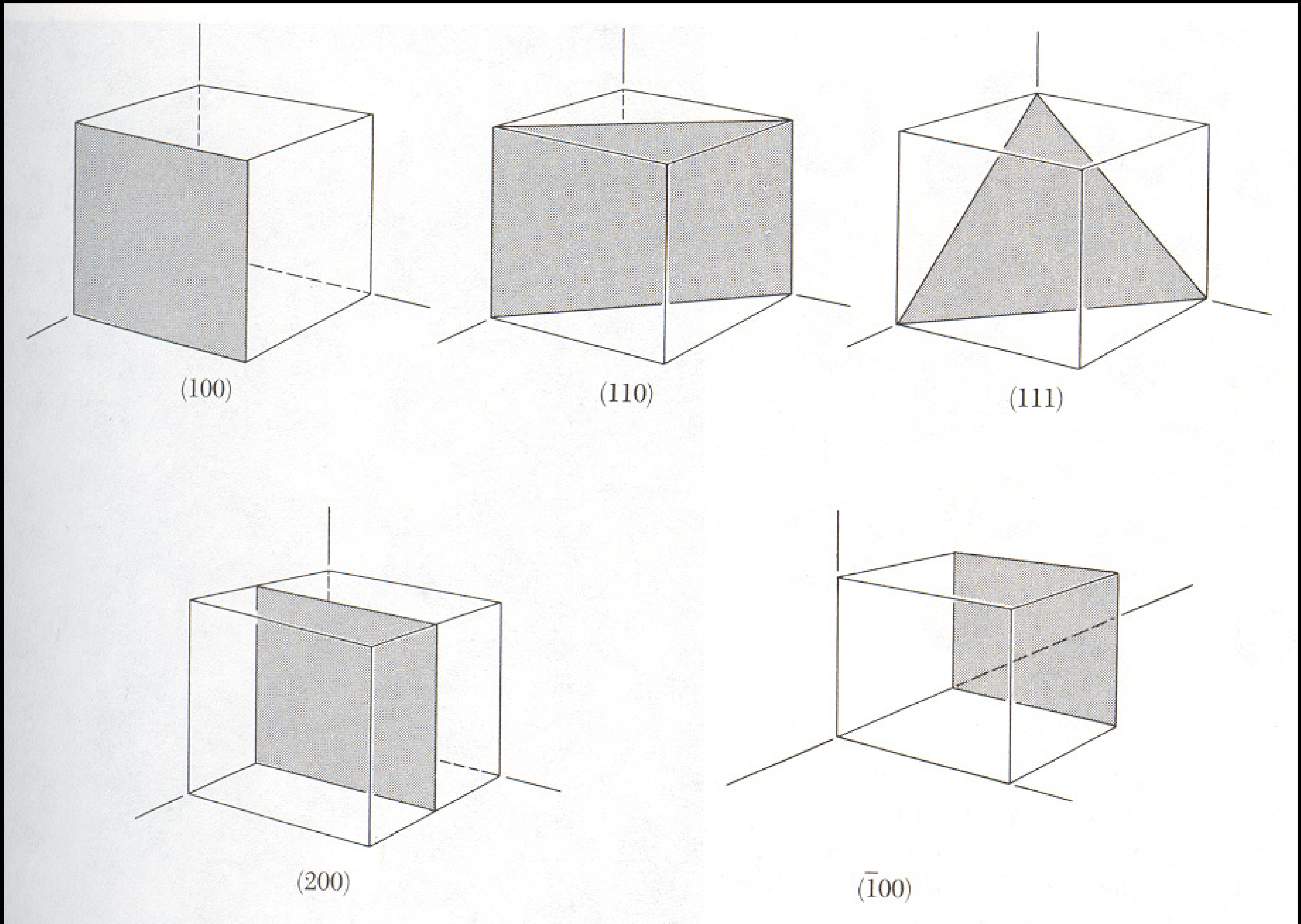
  u **a** , v **b**, w **c** is denoted by

  < **u v w** >**.**

- For all u v w positive the convention is **[u v w].**

- For say u negative the convention is **[ubar v w].**

Indices of planes in a cubic crystal



(100)

(110)

(111)

(200)

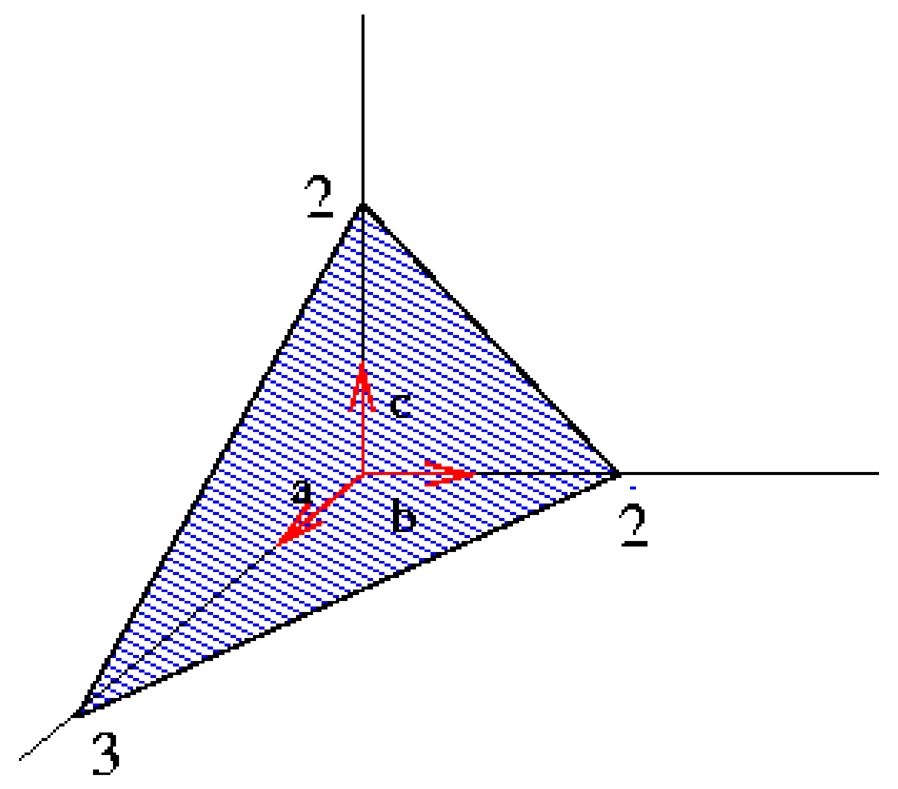
$(\bar{1}00)$

Miller Indices

- The orientation of a crystal plane is determined by 3 points in the plane, provided they are not collinear.

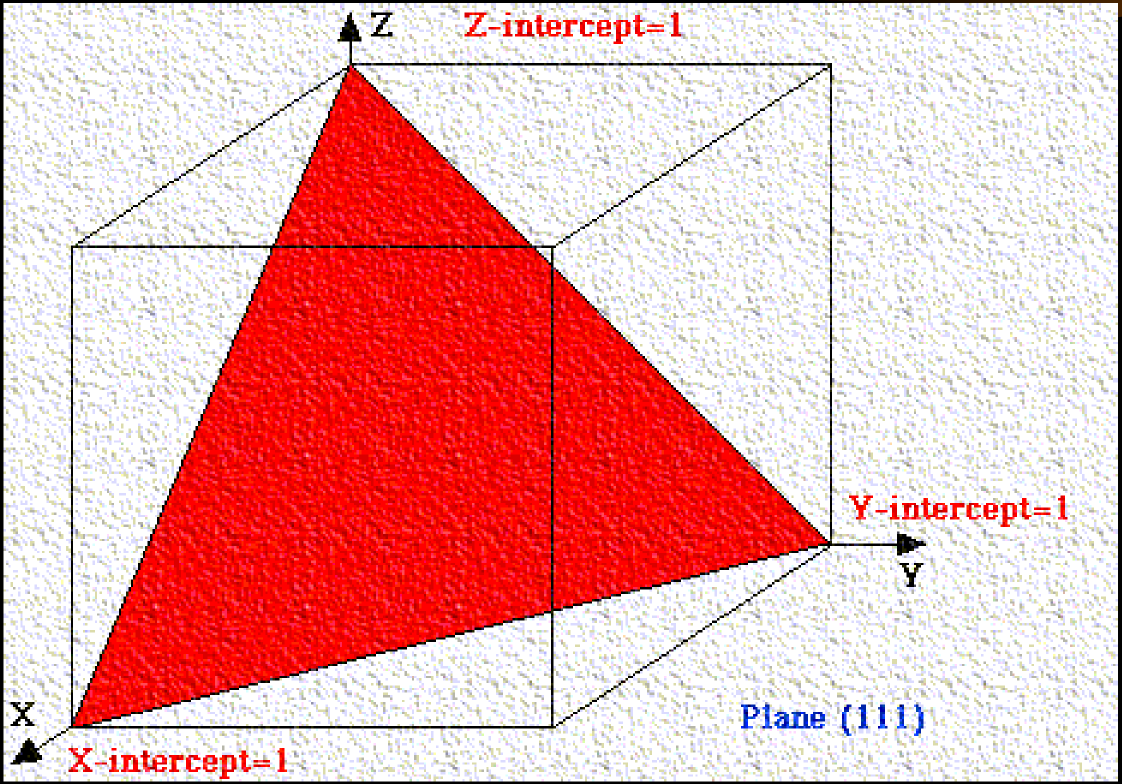
Rules:

- Find the intercept on the axes in terms of the lattice constants a, b, c. The axes may be those of a primitive or nonprimitive cell.
- Take the reciprocals of these numbers and then reduce to 3 integers having the same ratio, usually the smallest 3 integers. The result, (h k l), is called the **index of a plane**.
- **h, k, l** are known as ***Miller Indices***.



This plane intercepts the a, b, c axes at 3a, 2b, 2c. The reciprocals of these numbers are 1/3, 1/2, 1/2. So indices of the plane are **(2 3 3).**

Crystal Plane Animation



Spacing between Crystal planes

- It can be shown geometrically that the spacing d between planes of Miller indices {h k l} (curly brackets imply both +/- choices) in the cubic system is

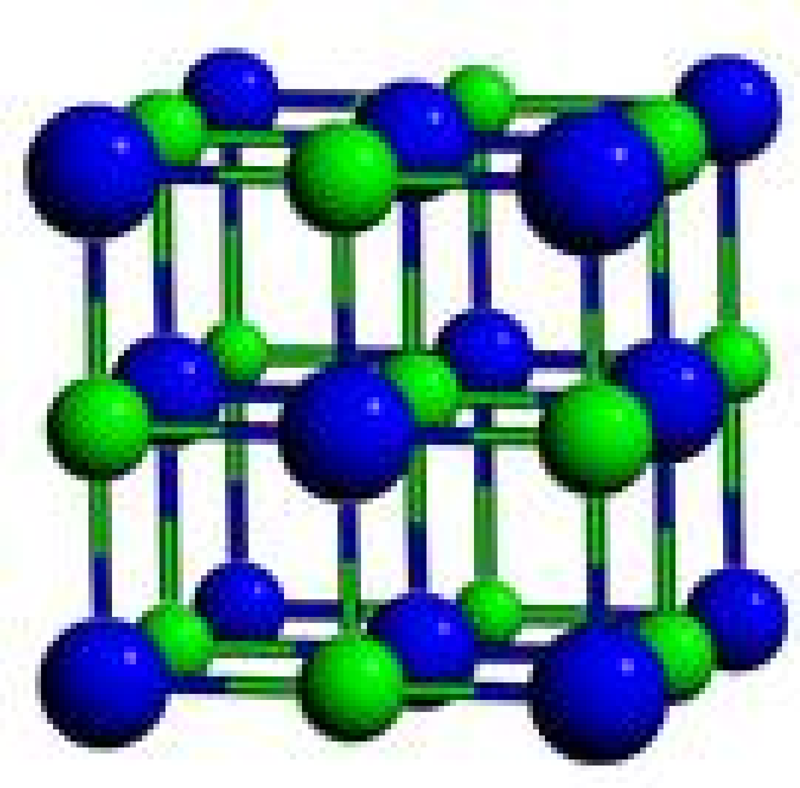
$$\mathbf{d = a / (h^2 + k^2 + l^2)^{1/2}.}$$

where **a** is the length of the edge of the cubic unit cell.

Simple Crystal Structures

Sodium Chloride Structure

- FCC lattice structure.
- The basis consists of one Na atom (green) and one Cl atom (blue) separated by one-half the body diagonal of a unit cube.



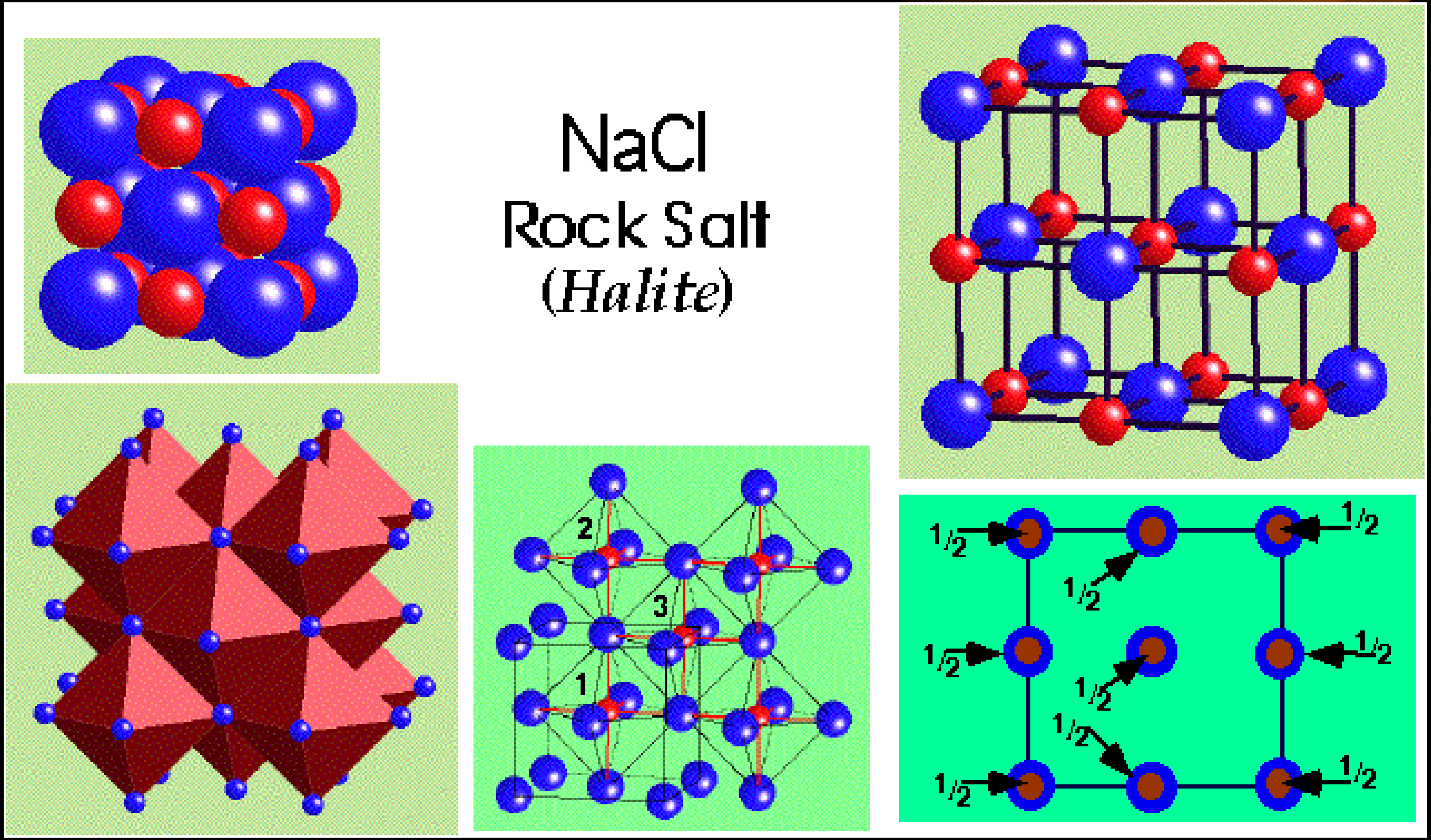
- There are 4 units of NaCl in each unit cube, with atoms in the positions

  Cl: 000; ½ ½ 0; ½ 0 ½; 0 ½ ½;

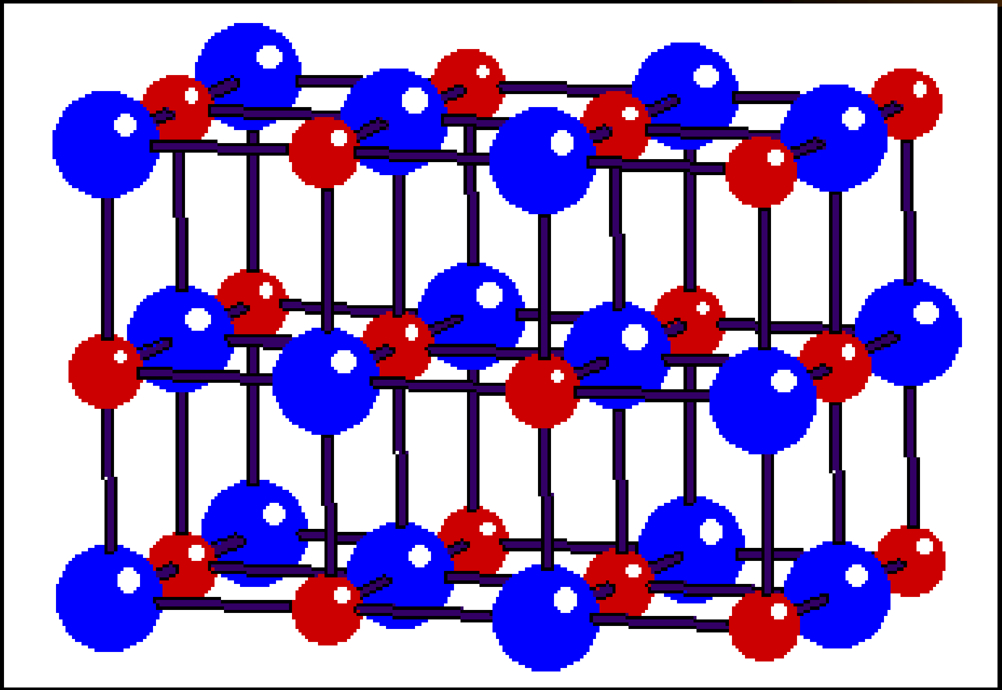
  Na:½ ½ ½; 00 ½; 0 ½ 0; ½0 0.

- Each atom has as nearest neighbors 6 atoms of opposite kind.
- Similar structures are LiH, MgO, MnO etc.

NaCl Rock Salt (Halite)



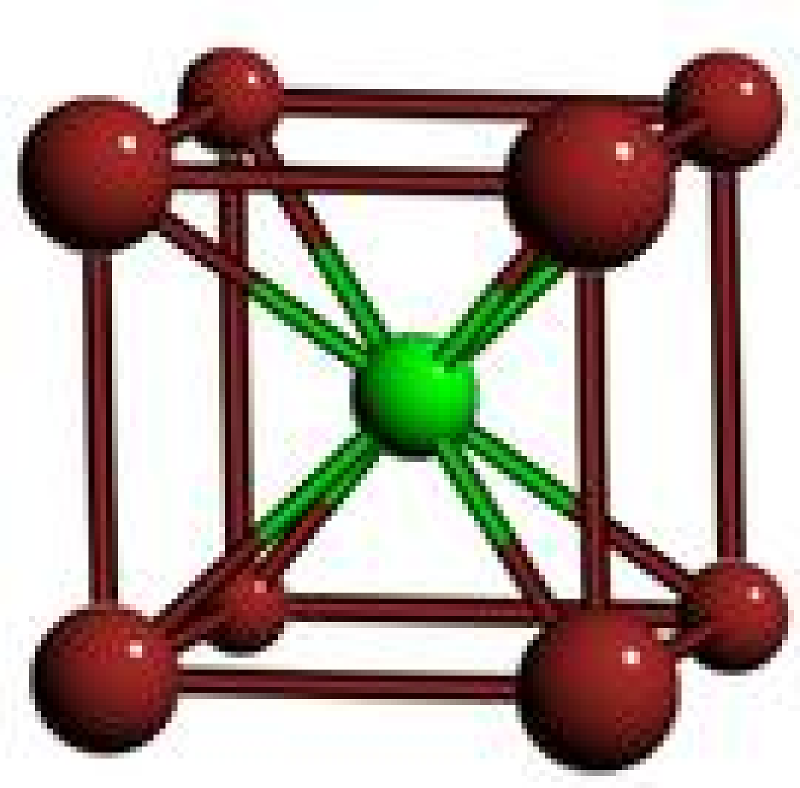
The fcc nature of the lattice can be seen by examining just one atom of the motif at a time (i.e. just Cl or just Na)



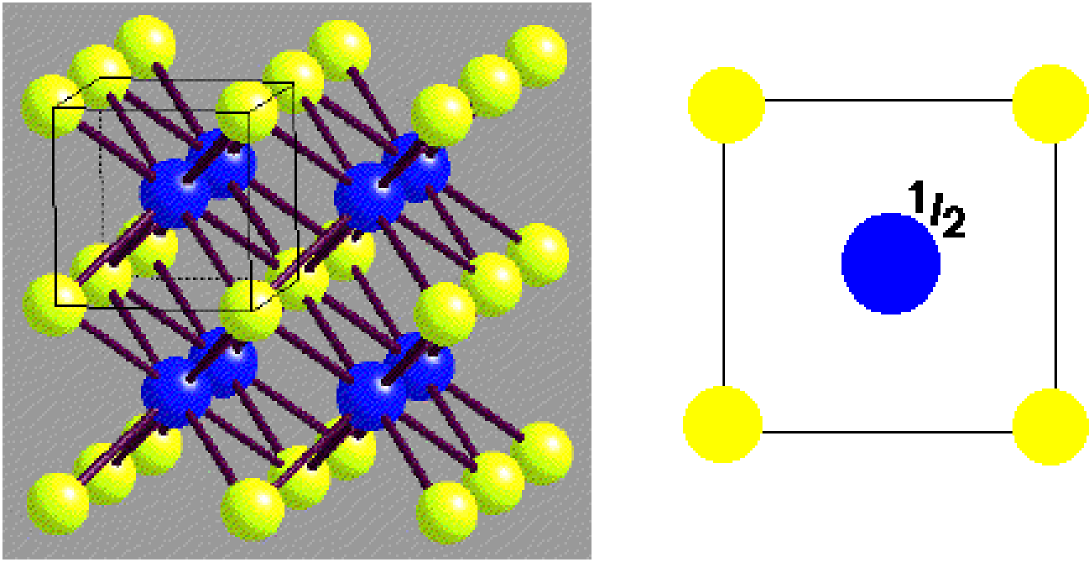
Cesium Chloride Structure

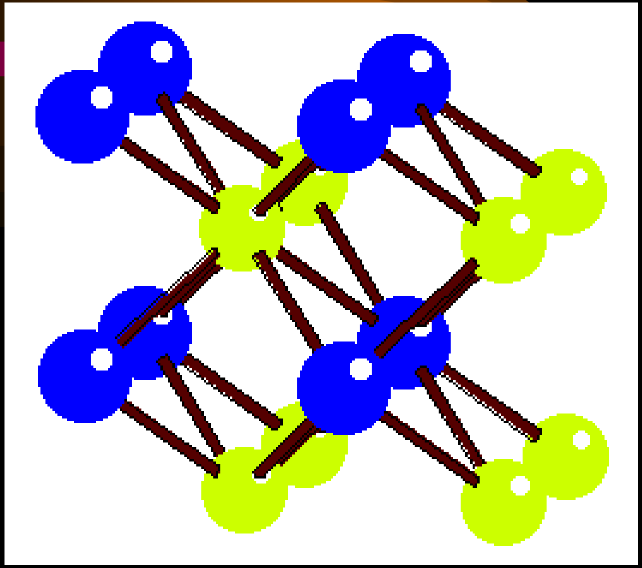
- BCC lattice structure.
- One molecule per primitive cell, with atoms at the corners 000 and body-centered positions

  ½ ½ ½ of the simple cubic space lattice.
- Coordination number is 8.
- Similar structures are BeCu, AlNi, CuZn, CuPd, AgMg etc.



CSCl Cesium Chloride Structure

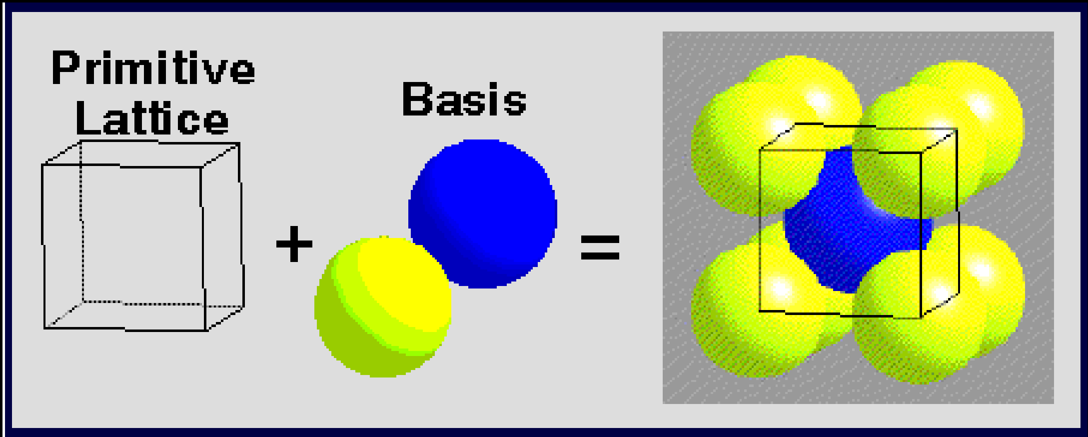




Lattice:

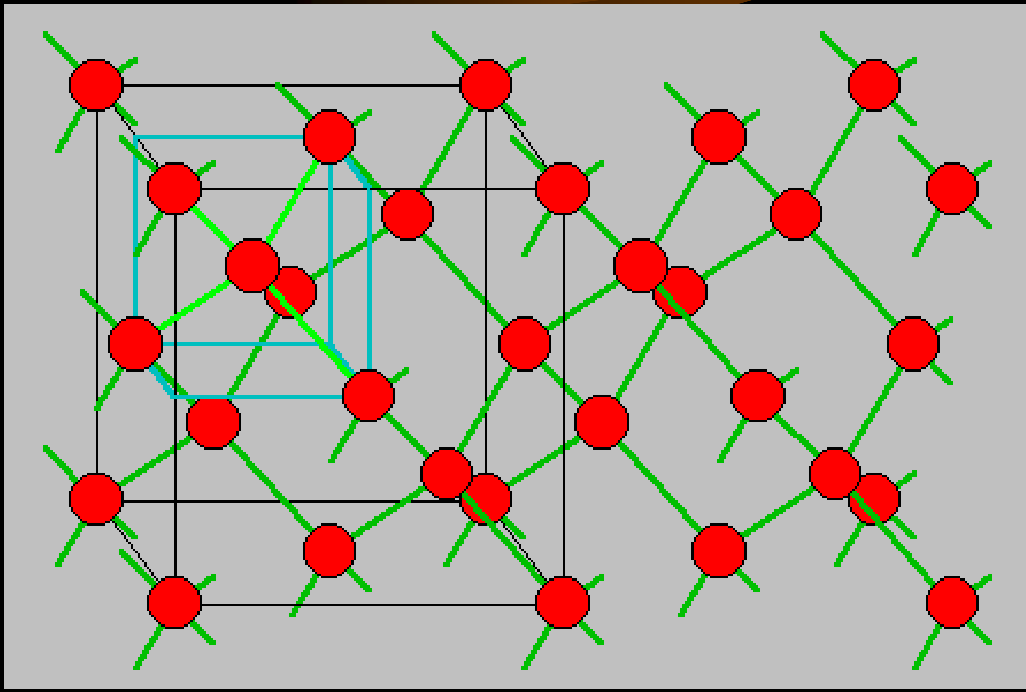
Cubic – P

(Primitive)



Diamond Structure

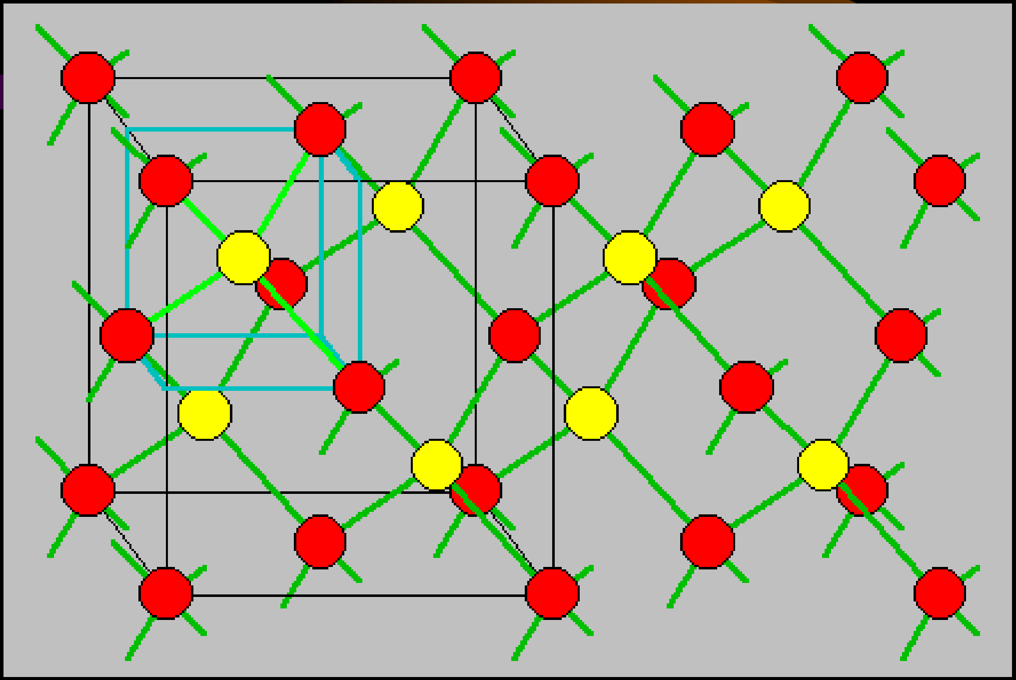
- Space lattice is FCC.
- Primitive basis has two identical atoms at 000; ¼ ¼ ¼ associated with each point of the fcc lattice.
- Each atom has 4 nearest neighbors and 12 next nearest neighbors.
- The diamond lattice represents the crystal structure of diamond, germanium and silicon.



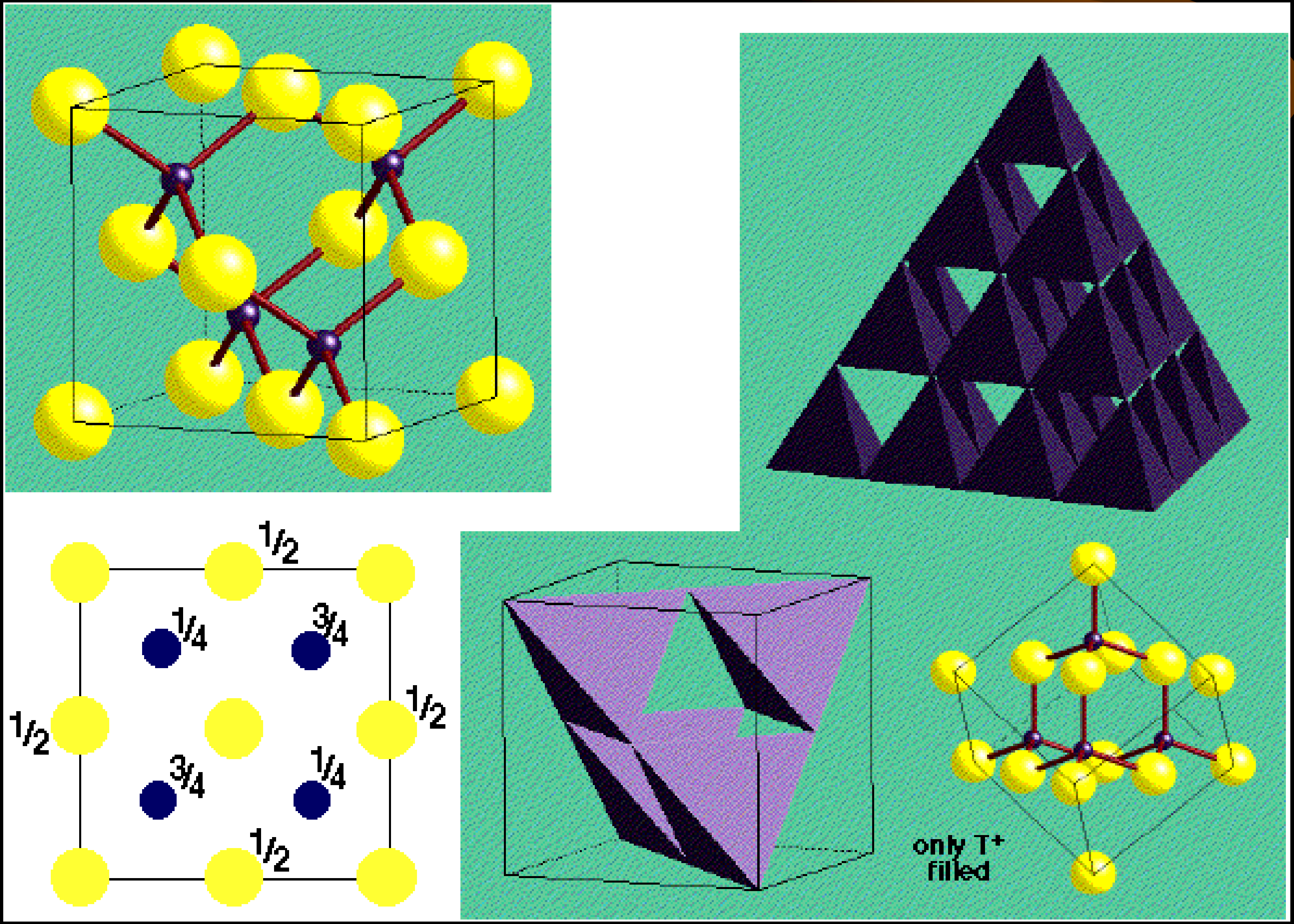
Zincblende Structure

- The zincblende lattice consist of a face centered cubic Bravais point lattice which contains two different atoms per lattice point. The distance between the two atom equals one quarter of the body diagonal of the cube.

- The zincblende lattice represents the crystal structure of zincblende (ZnS), gallium arsenide, indium phosphide, cubic silicon carbide and cubic gallium nitride.



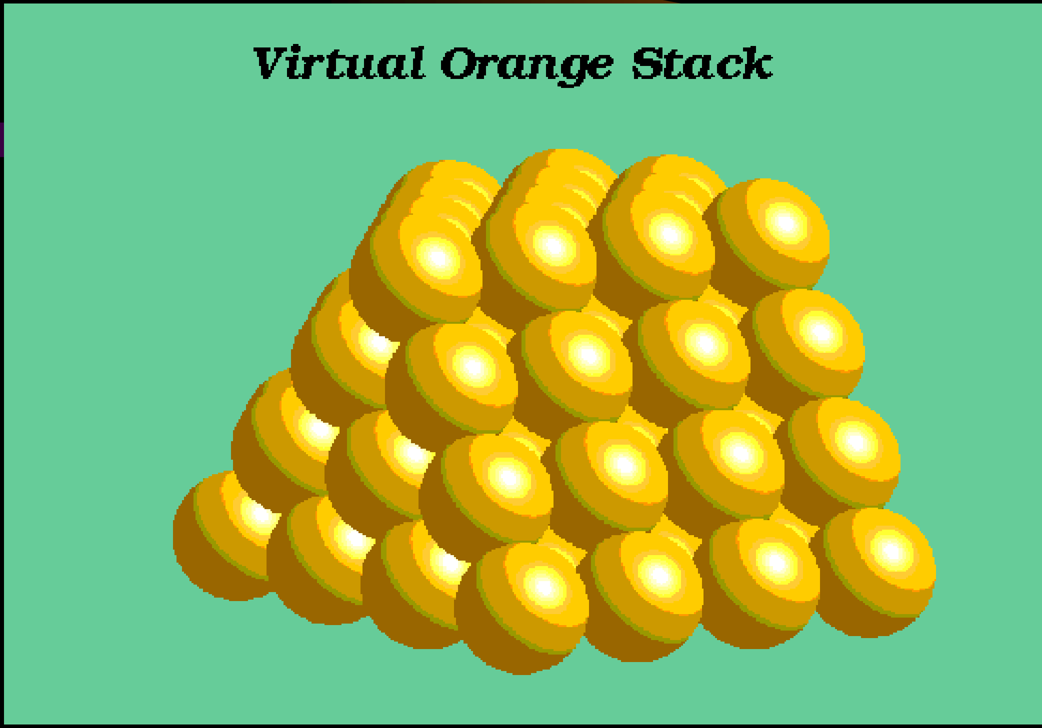
ZnS Zinc Blende (Sphalerite)



Close-packed Structure

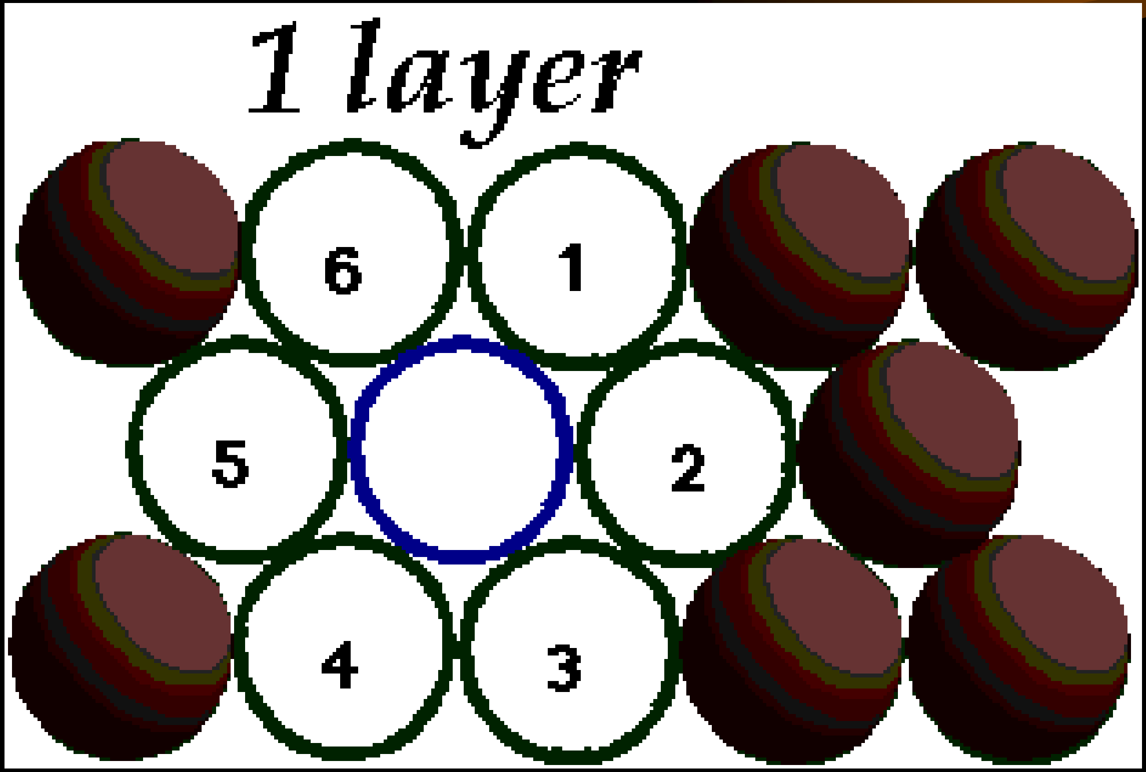
- Goldschmidt proposed that atoms could be considered as packing in solids as hard spheres.

- This reduces the problem of examining the packing of like atoms to that of examining the most efficient packing of any spherical object.



Have you noticed how oranges are most effectively packed in displays at your local shop?

Close-packing of spheres



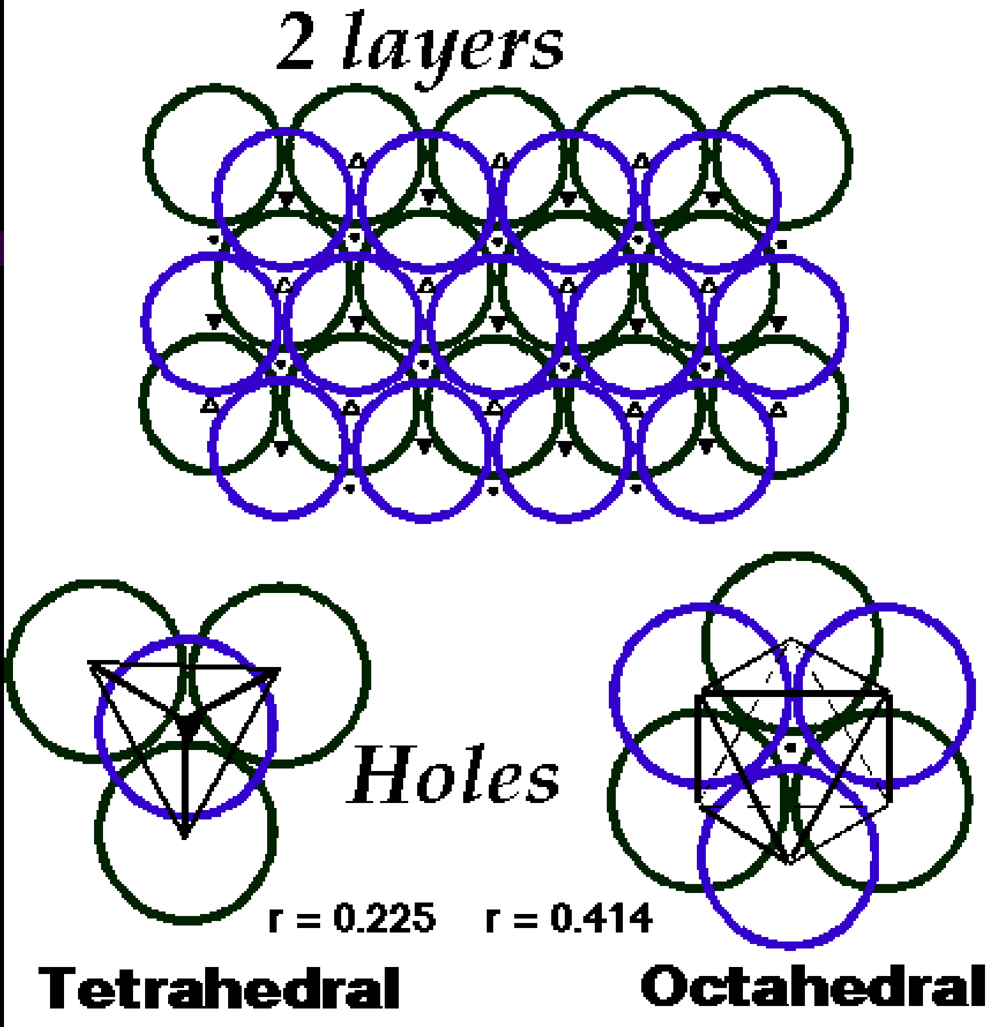
A ***single*** layer of spheres is closest-packed with a HEXAGONAL coordination of each sphere

A ***second*** layer of spheres is placed in the indentations left by the first layer

- space is trapped between the layers that is not filled by the spheres
- TWO different types of **HOLES** (so-called **INTERSTITIAL** sites) are left :

  OCTAHEDRAL (O) holes with 6 nearest sphere neighbours and

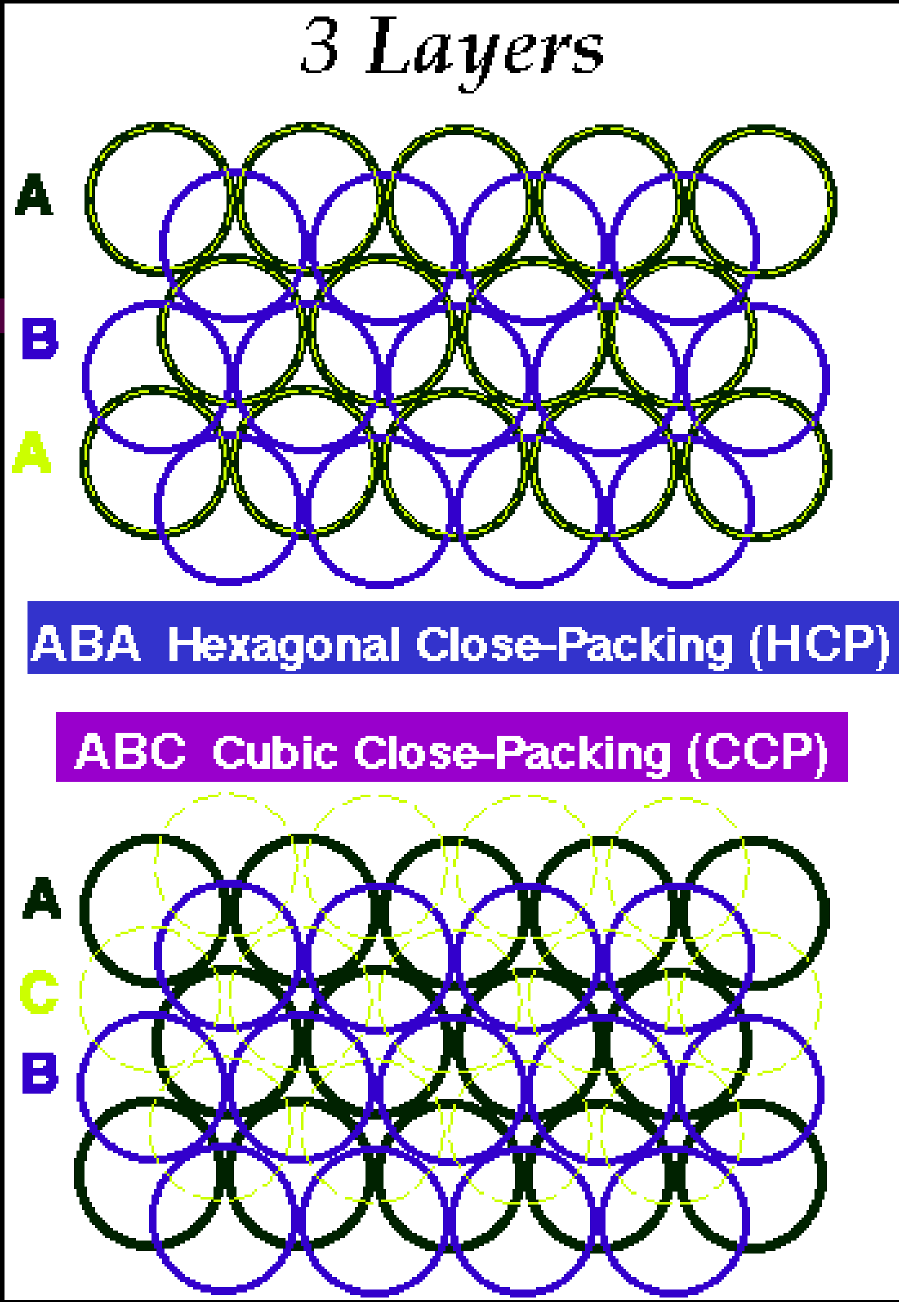
  TETRAHEDRAL (T±) holes with 4 nearest sphere neighbours.



- When a ***third*** layer of spheres is placed in the indentations of the second layer there are **TWO** choices:

- The third layer lies in indentations directly in line (eclipsed) with the 1st layer. Layer ordering may be described as **ABA.**

- The third layer lies in the alternative indentations leaving it staggered with respect to both previous layers. Layer ordering may be described as ABC.



Simplest close-packing structures

- **ABABAB**.... repeat gives **Hexagonal Close-Packing (HCP)**

  Unit cell showing the full symmetry of the arrangement is ***Hexagonal***

  Hexagonal: $a = b$, $c = 1.63a$, $\alpha = \beta = 90°$, $\gamma = 120°$

  2 atoms in the unit cell: (0, 0, 0) ; (2/3, 1/3, 1/2)

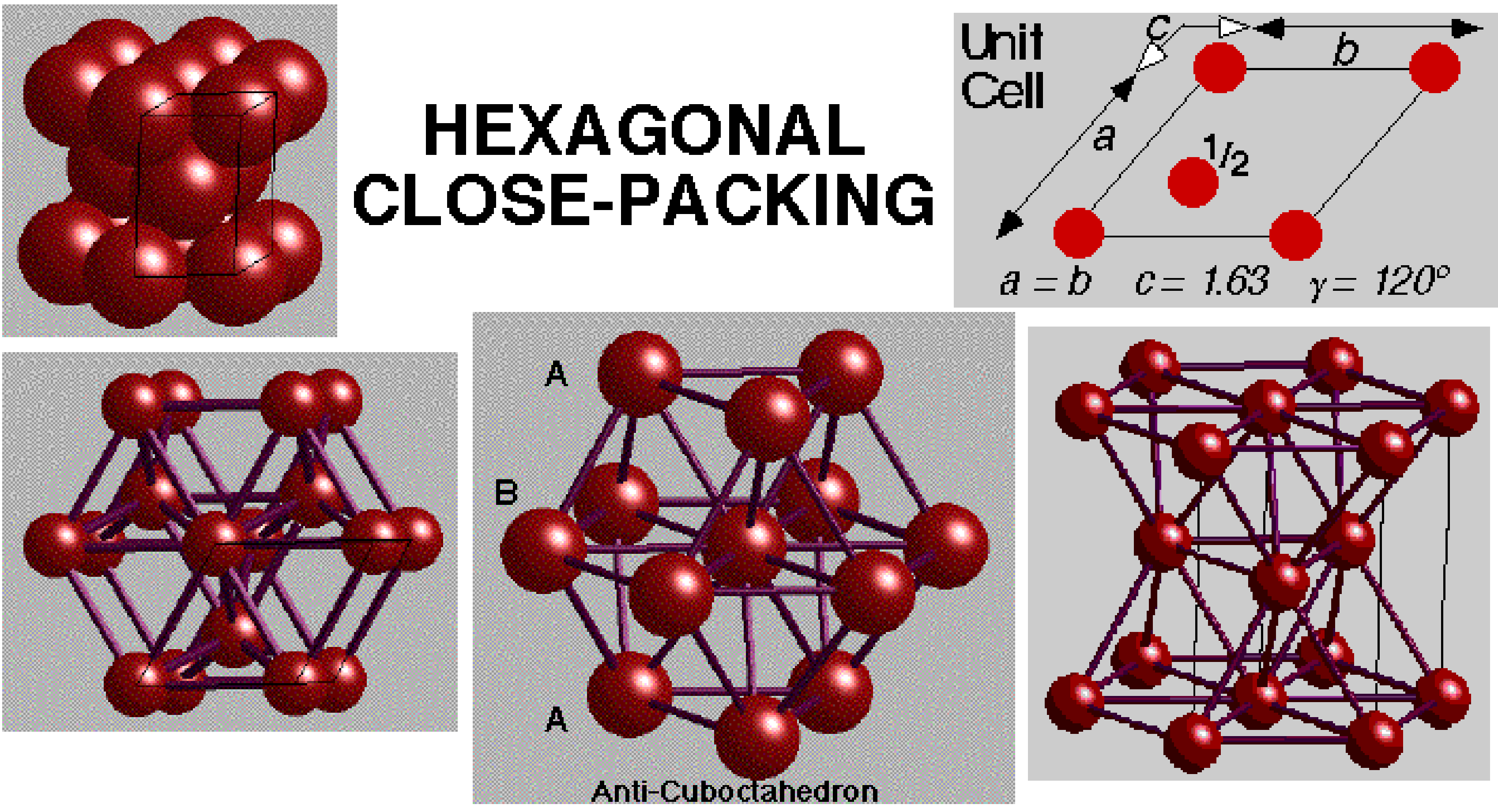
- **ABCABC**.... repeat gives **Cubic Close-Packing (CCP)**

  Unit cell showing the full symmetry of the arrangement is ***Face-Centred Cubic***

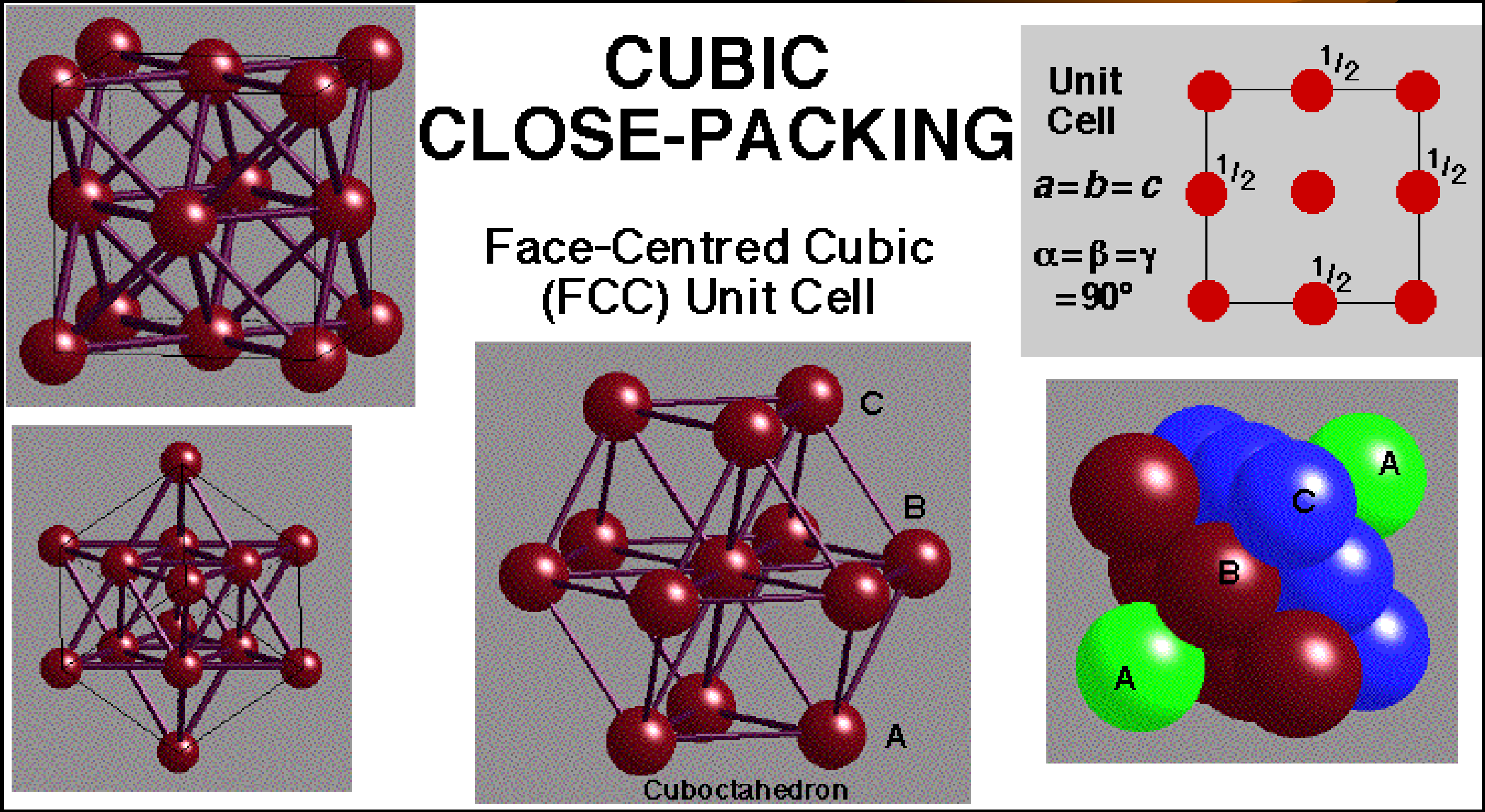
  Cubic: $a = b = c$, $\alpha = \beta = \gamma = 90°$

  4 atoms in the unit cell: (0, 0, 0); (0, 1/2, 1/2) ; (1/2, 0, 1/2); (1/2, 1/2, 0)

HCP Structure



CCP Structure

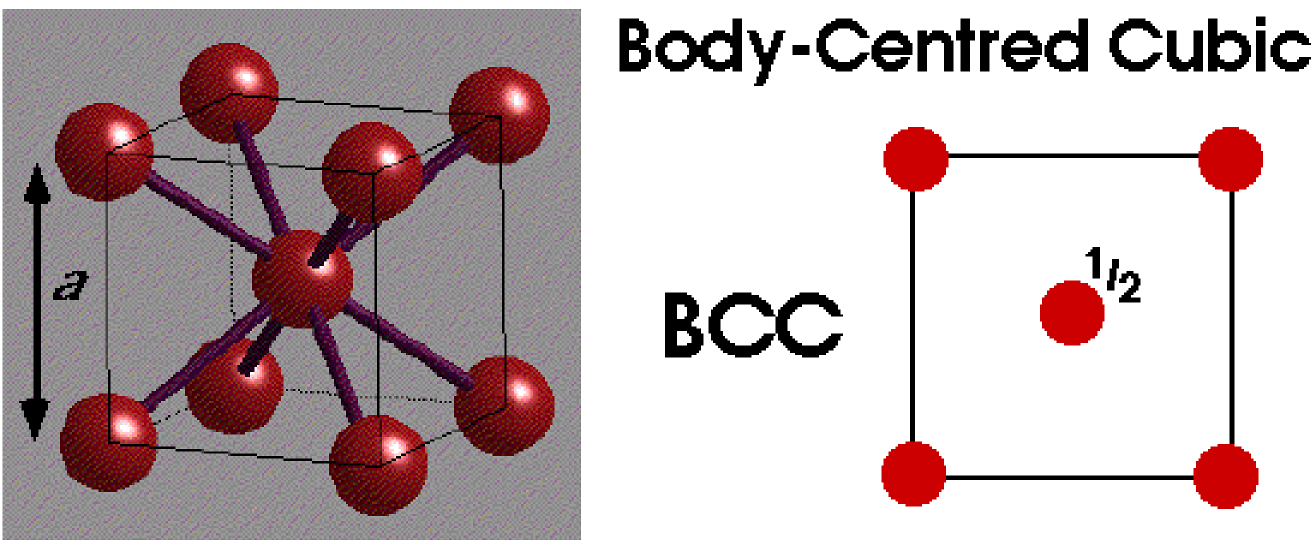


CUBIC CLOSE-PACKING

Face-Centred Cubic (FCC) Unit Cell

The **most common close-packed structures** are **METALS**

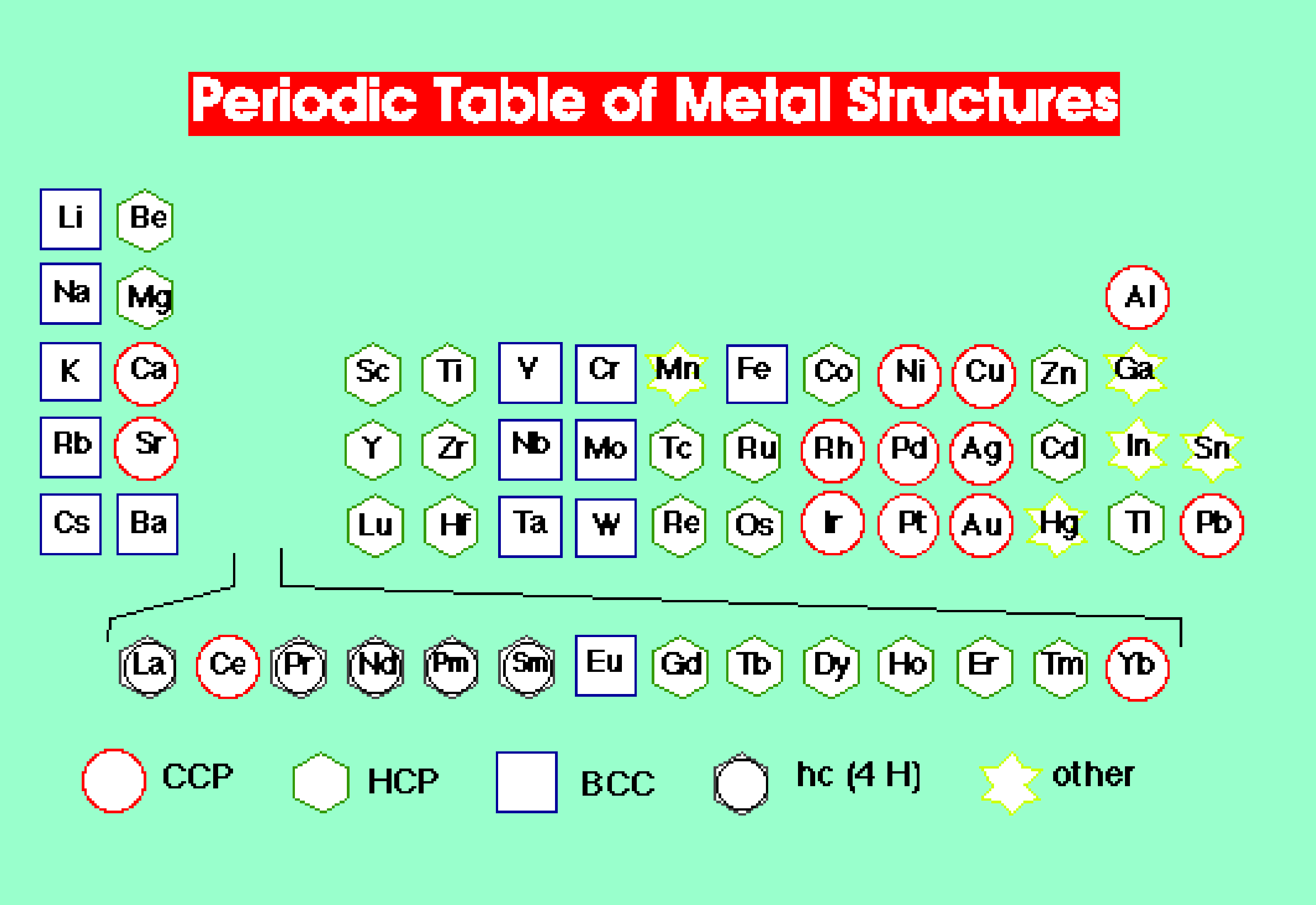
A NON-CLOSE-PACKED structure adopted by some metals is:



68% of space is occupied.

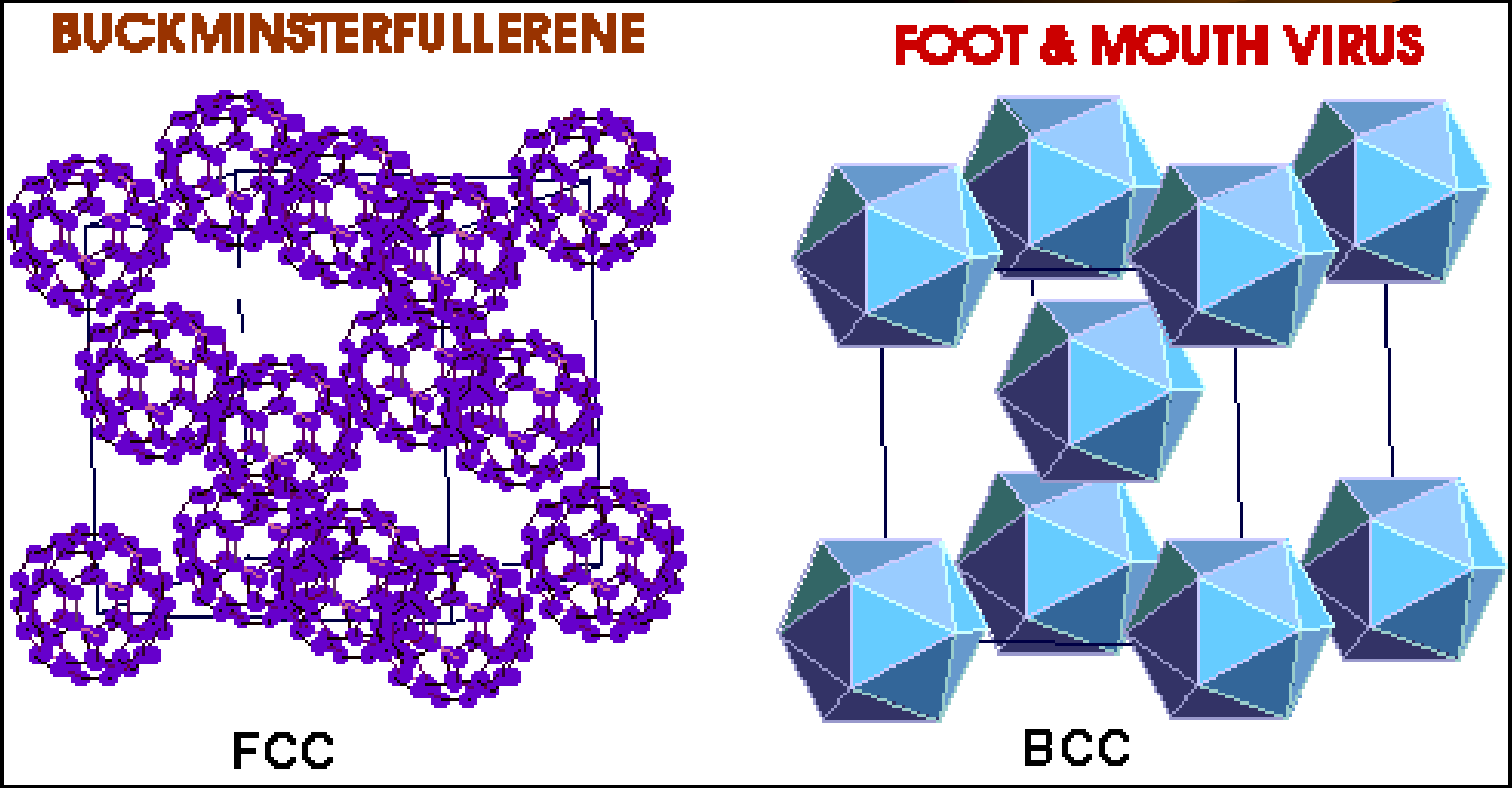
Coordination Number ?

8 Nearest Neighbours at **0.87a** and 6 Next-Nearest Neighbours at **1a.**



- ***Polymorphism:*** Some metals exist in different structure types at ambient temperature & pressure.
- Many metals adopt different structures at different temperature/pressure.
- *Not all metals are close-packed*.

Other systems may be Classified as having Similar Structures



Reciprocal Lattice

Definition

- Consider a set of points **R** constituting a Bravais lattice (B. L), and a plane wave, exp(i**k.r**). For general **k**, such a plane wave will not, of course, have the periodicity of the B. L, but for certain special choices of **k** it will.

- The set of all wave vectors **K** that yield plane waves with the periodicity of a given B. L is known as its ***reciprocal vector***.

- Mathematically, **K** belongs to the reciprocal lattice of a B. L of points **R**, provided that the relation

  $$\exp(i\,\mathbf{K}.(\mathbf{r}+\mathbf{R})) = \exp(i\,\mathbf{K}.\mathbf{r})$$

  holds for any **r**, and for all **R** in the B. L.

- So we can characterize the reciprocal lattice as the set of wave vectors **K** satisfying

  $$\exp(i\,\mathbf{K}.\mathbf{R}) = 1 \text{ for all } \mathbf{R} \text{ in the B. L.}$$

Properties of Reciprocal Lattice

- The reciprocal lattice is a B. L.
- If $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ are a set of primitive vectors for a direct lattice then the reciprocal lattice can be generated by the three primitive vectors

$$\mathbf{b}_1 = 2\pi\, (\mathbf{a}_2 \times \mathbf{a}_3)/(\mathbf{a}_1 . (\mathbf{a}_2 \times \mathbf{a}_3)),$$

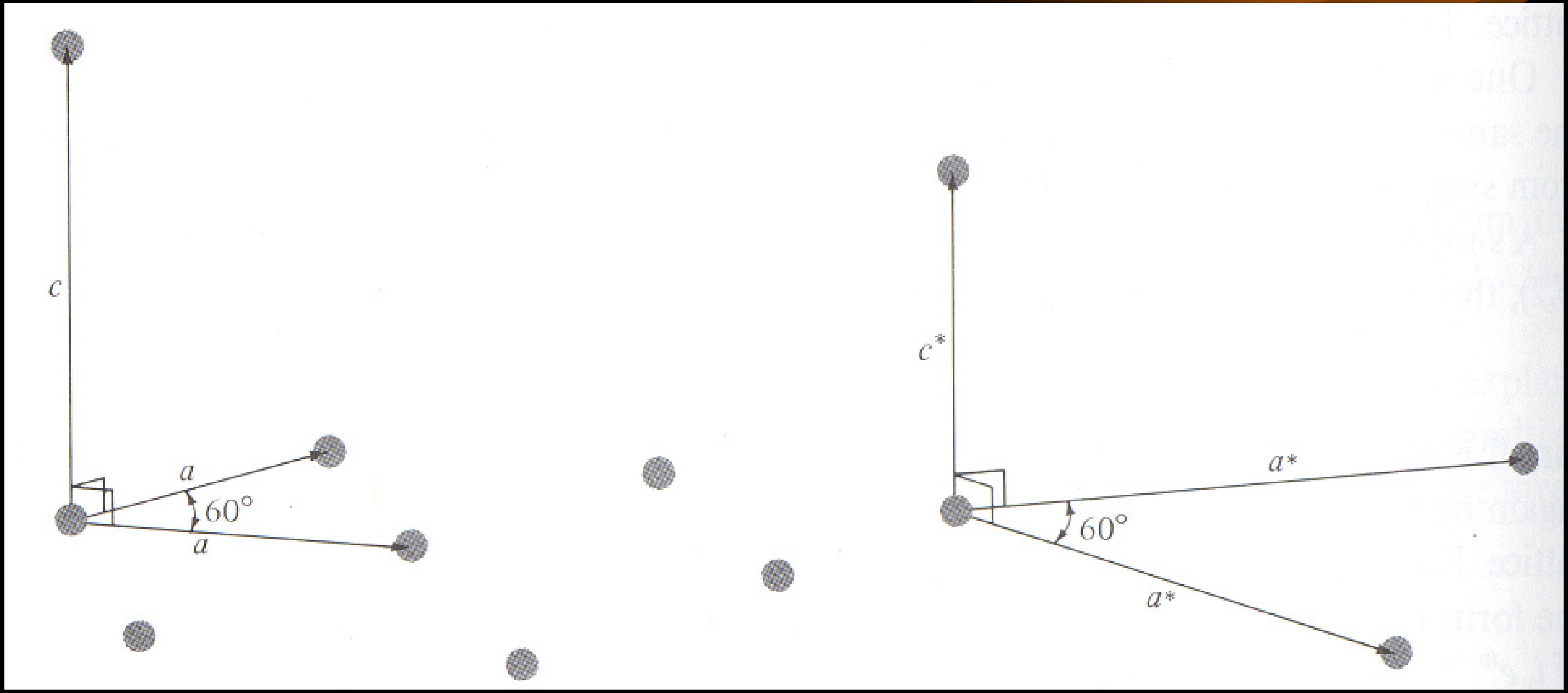
$$\mathbf{b}_2 = 2\pi\, (\mathbf{a}_3 \times \mathbf{a}_1)/(\mathbf{a}_1 . (\mathbf{a}_2 \times \mathbf{a}_3)),$$

$$\mathbf{b}_3 = 2\pi\, (\mathbf{a}_1 \times \mathbf{a}_2)/(\mathbf{a}_1 . (\mathbf{a}_2 \times \mathbf{a}_3)).$$

- Note that $\mathbf{b}_i . \mathbf{a}_j = 2\pi\delta_{ij}$.
- Any vector k can be written as $\mathbf{k} = \mathbf{k}_1\mathbf{b}_1 + \mathbf{k}_2\mathbf{b}_2 + \mathbf{k}_3\mathbf{b}_3$.
- If R is any direct lattice vector, then $\mathbf{R} = \mathbf{n}_1\mathbf{a}_1 + \mathbf{n}_2\mathbf{a}_2 + \mathbf{n}_3\mathbf{a}_3$.
- Check that $\mathbf{k.R} = 2\pi(\mathbf{k}_1\mathbf{n}_1+\mathbf{k}_2\mathbf{n}_2+\mathbf{k}_3\mathbf{n}_3) = 2\pi \times$ integer.

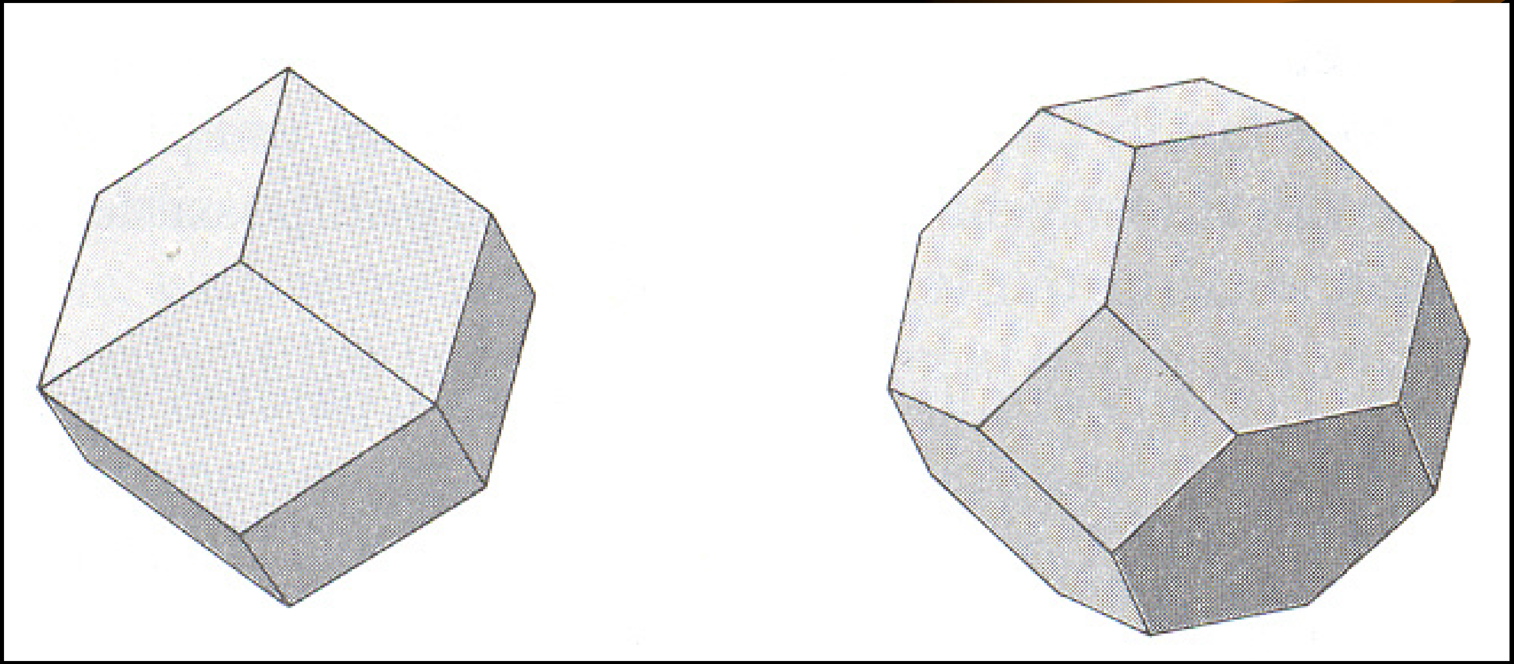
  So, $\exp(i\, \mathbf{k.R}) = 1$.

Examples



Primitive vectors for the simple hexagonal Bravais lattice (Left)
Primitive vectors for the corresponding reciprocal lattice (Right)

First Brillouin Zone



The Wigner-Seitz primitive cell of the reciprocal lattice is known as the first Brillouin zone.

Left: First BZ for BCC lattice **Right:** First BZ for FCC lattice

Reciprocal lattice vectors and Real space planes

- If a plane in real space has Miller indices (***h k l***) then the reciprocal lattice vector

  $$\mathbf{K} = h\,\mathbf{b}_1 + k\,\mathbf{b}_2 + l\,\mathbf{b}_3$$

  is perpendicular to it.

- The spacing **d(*hkl*)** between parallel lattice planes that are normal to the direction **K** is

  $$\mathbf{d}(hkl) = 2\pi/|\mathbf{K}|.$$

Interplanar Spacing ***d****:*

$$V = abc(1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma)^{1/2}$$

$$a^* = V^{-1}bc\sin\alpha$$

$$b^* = V^{-1}ac\sin\beta$$

$$c^* = V^{-1}ab\sin\gamma$$

$$V^* = V^{-1}$$

$$\frac{1}{d^2} = \frac{h^2}{a^2}+\frac{k^2}{b^2}+\frac{l^2}{c^2} \quad \text{(orthogonal)}$$

$$\frac{1}{d^2} = \frac{4}{3}\cdot\frac{h^2+k^2+hk}{a^2}+\frac{l^2}{c^2} \quad \text{(hexagonal)}$$

$$\frac{1}{d^2} = \frac{\left(\begin{array}{l}\dfrac{h^2}{a^2}\sin^2\alpha+\dfrac{k^2}{b^2}\sin^2\beta+\dfrac{l^2}{c^2}\sin^2\gamma+ \\ +\dfrac{2kl}{bc}(\cos\beta\cos\gamma-\cos\alpha)+ \\ +\dfrac{2hl}{ac}(\cos\alpha\cos\gamma-\cos\beta)+\dfrac{2hk}{ab}(\cos\alpha\cos\beta-\cos\gamma)\end{array}\right)}{(1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma)} \quad \text{(triclinic)}$$

Diffraction of waves by crystals

Scattering of x rays by a perfect periodic structure

Two equivalent views:

- ***Bragg Formulation of X-ray diffraction by a crystal*** – widely used by x-ray crystallographers.
- ***von Laue approach*** – exploits the reciprocal lattice. This approach is closer to the spirit of modern solid state physics.
- Note: Both formulations are equivalent.

Bragg formulation of x-ray diffraction by a crystal

Rays interfere constructively if

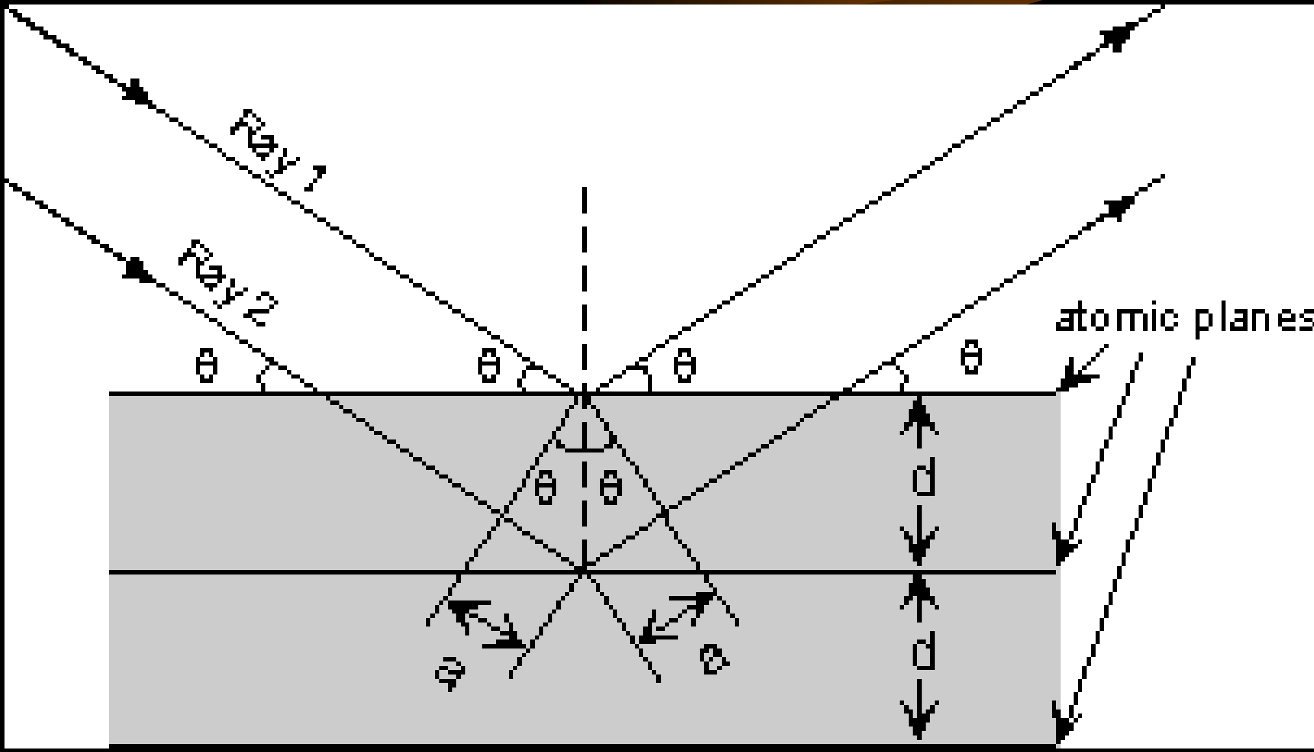
$$2a = m\lambda$$

Now

$$a = d \sin\theta.$$

Bragg's law of diffraction:

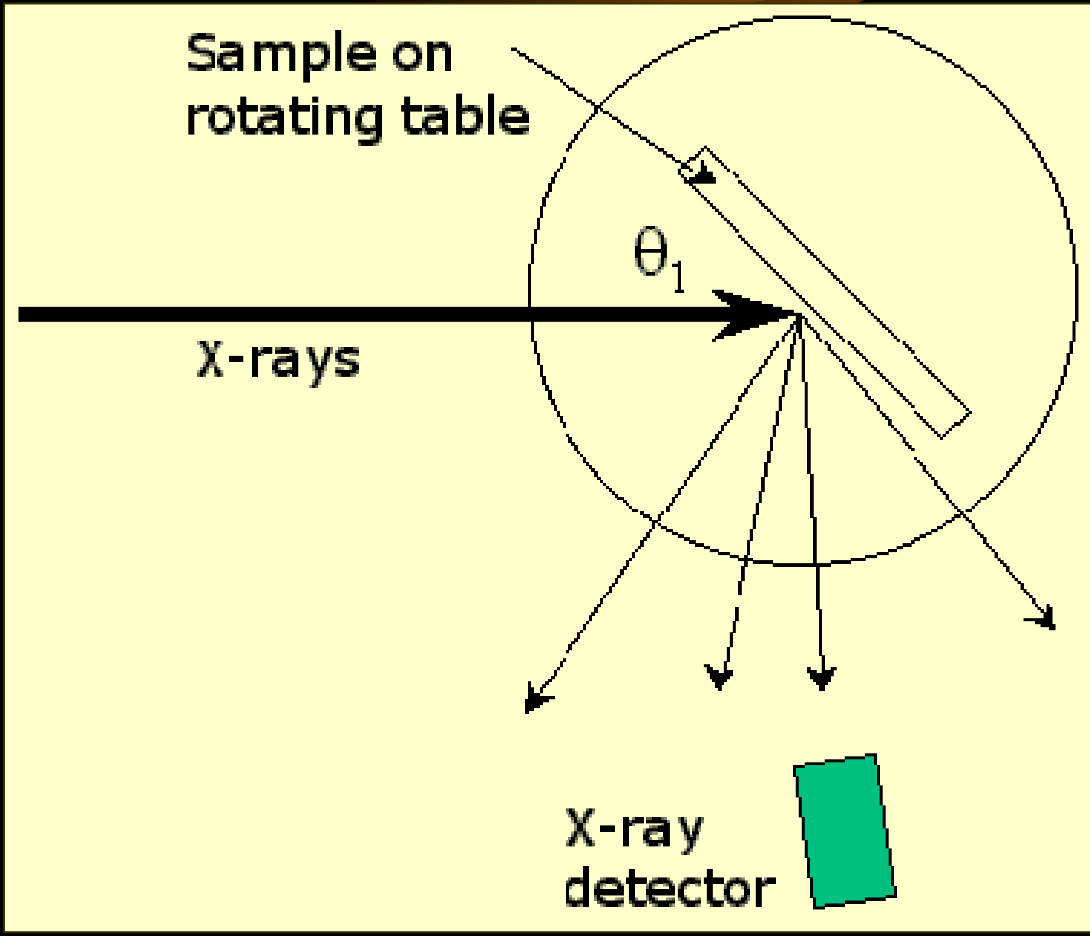
$$2d\sin\theta = m\lambda$$



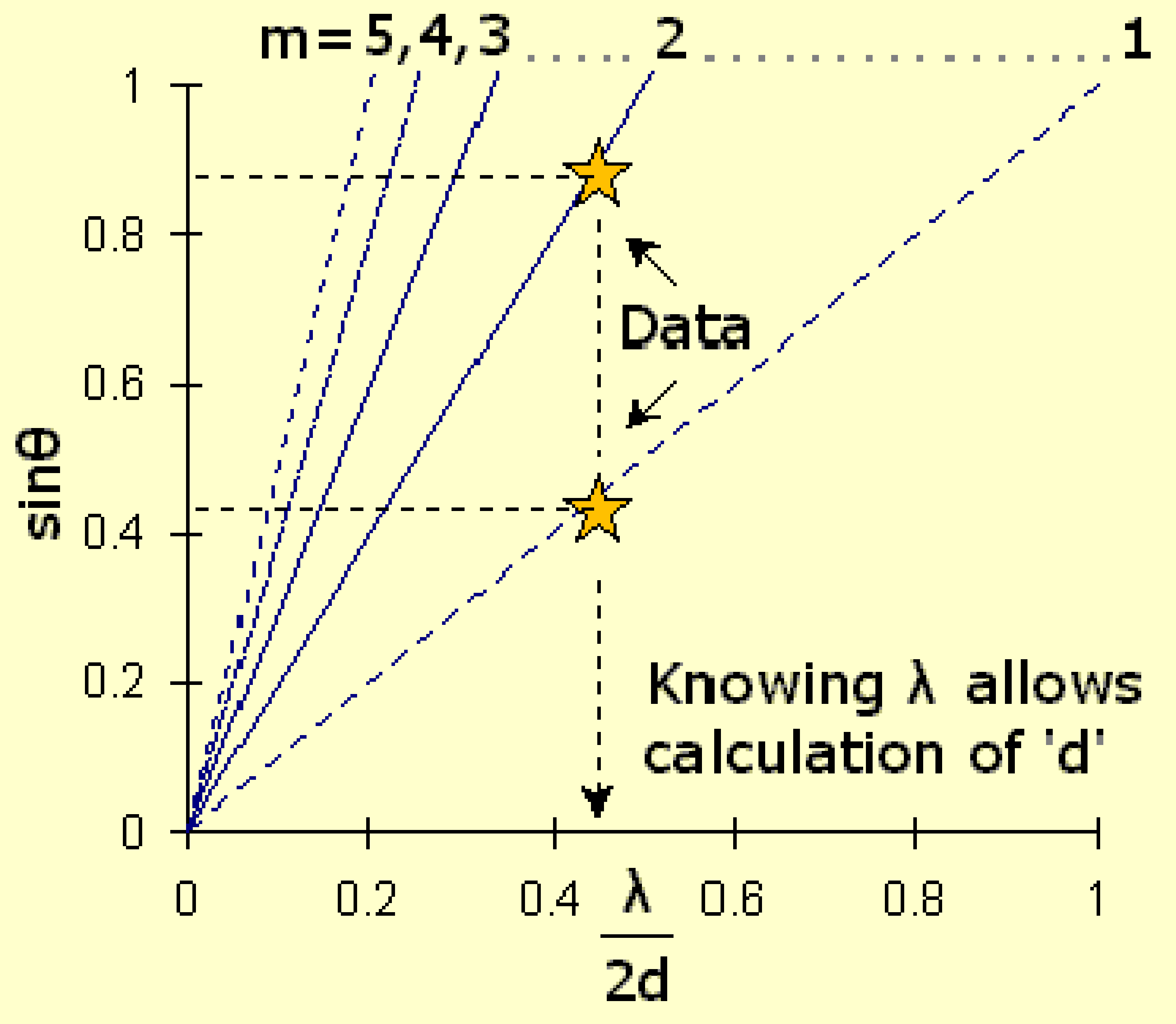
How do we perform an experiment?

- Measure angle and intensity of radiation as the table is rotated.
- Apply Bragg’s law

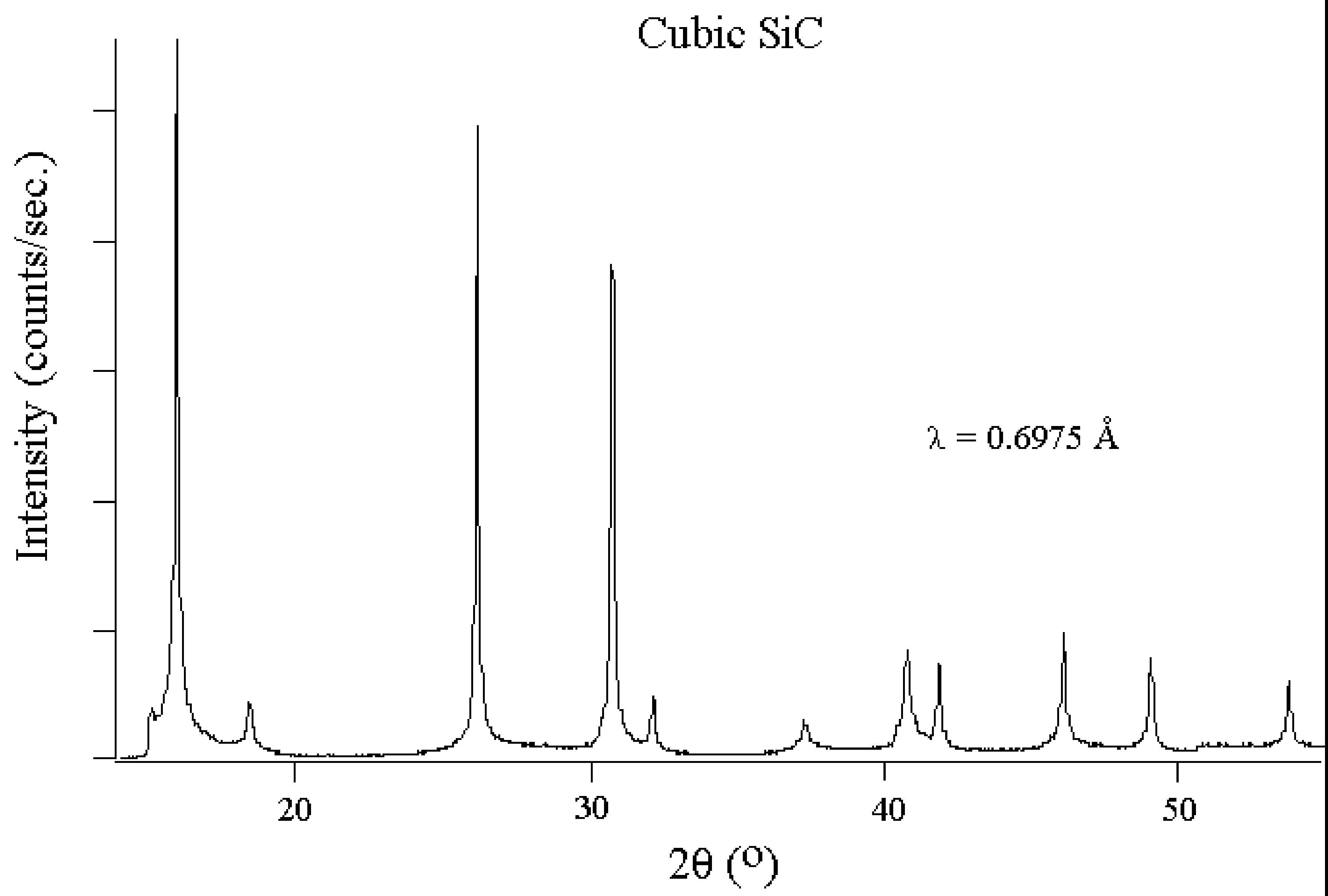
$$2d\sin\theta = m\lambda$$



Result:


m = 5, 4, 3
2
1
1
0.8
0.6
0.4
0.2
0
sinθ
0
0.2
0.4
0.6
0.8
1
λ
2d
Data
Knowing λ allows calculation of 'd'

Data



Atomic Scattering Factor

- The incoming X-rays are scattered by the electrons of the atoms.
- We define a quantity *f*, the **atomic scattering factor**. It describes the “efficiency” of scattering of a given atom in a given direction:

f = (amplitude of the wave scattered by an atom)/(amplitude of the wave scattered by one electron).

f decreases with increase in θ. For $\theta = 0$, $f = Z$ for any atom. (**Z**=atomic number).

Structure Factor

- Resultant wave scattered by all the atoms of the unit cell is called the structure factor, as it describes how the atom arrangement, given by **uvw** of each atom, affects the scattered beam.

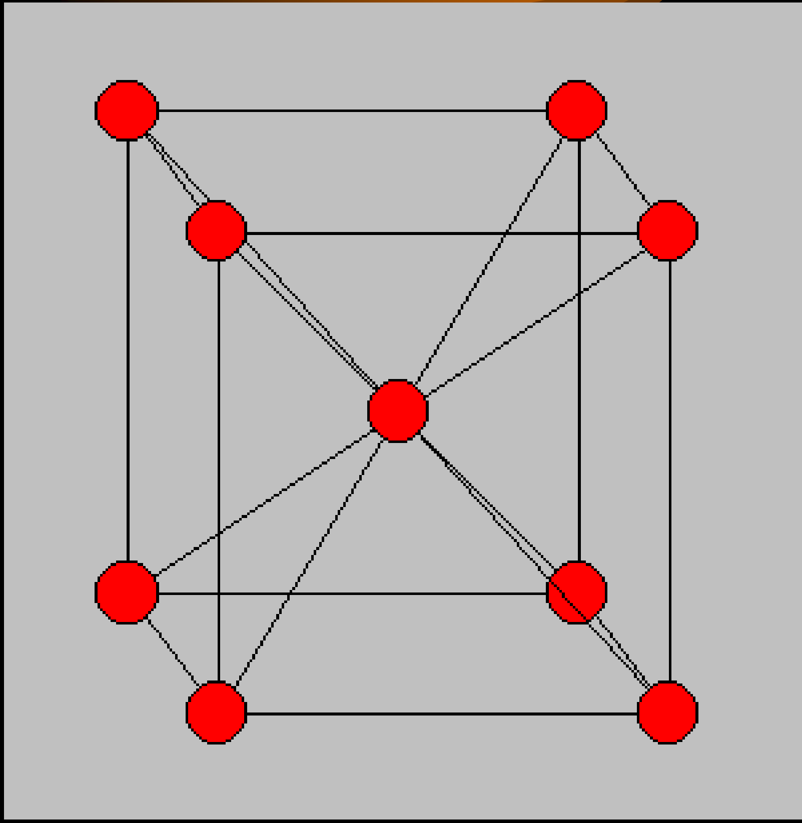
$$F_{(h,k,l)} = \sum_{j=1}^{atoms} f_{(j)} \exp\left[2\pi \cdot i(hx_{(j)} + ky_{(j)} + lz_{(j)})\right]$$

- The **intensity** is directly related to the structure factor:

$$I_{hkl} = \left|F_{hkl}\right|^2 \cdot LP \cdot A$$

where the factor **LP** is a combined geometry and polarization factor which depends on the particular experimental setup.

Example: BCC lattice



- It has two identical atoms per unit cell located at **000** and ½ ½ ½ . So,

$F = f\,[\, e^{2\pi i(0)} + e^{2\pi i(h/2+k/2+l/2)}\,]$

$= f\,[1 + e^{\pi i(h+k+l)}]$.

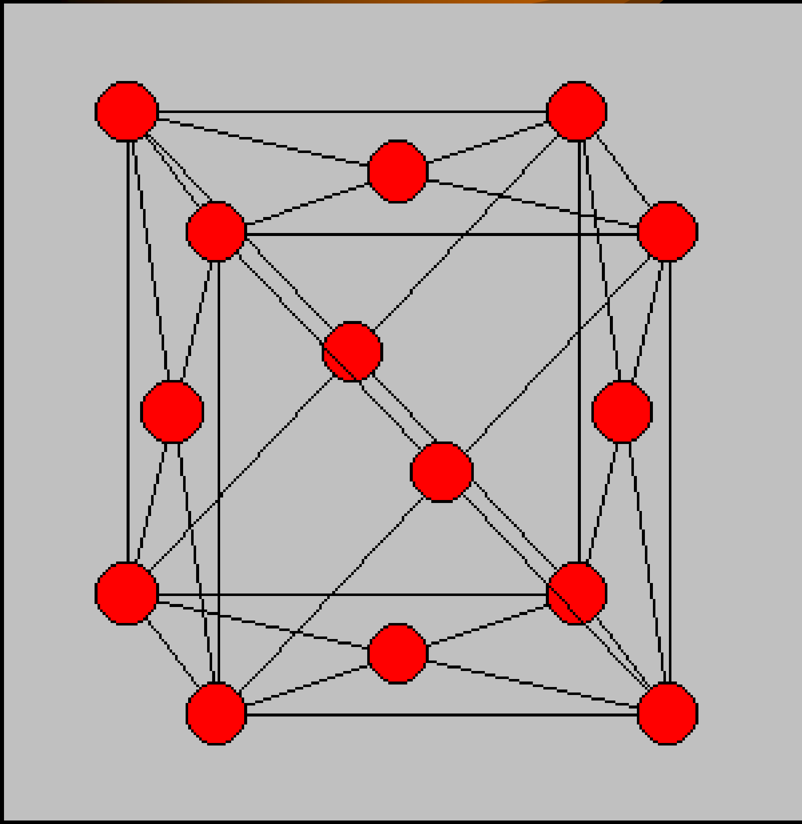
$F = 2f$, $|F|^2 = 4f^2$ when **(h+k+l)** is **even;**

$F = 0$, $|F|^2 = 0$ when **(h+k+l)** is **odd.**

=> In the diffraction pattern ***no reflections occur*** for planes **(100), (300), (111), (221)** etc. ***but reflections may occur*** for planes **(200), (110), and (222)** .

Example: FCC lattice

- It has identical atoms per unit cell at **000, 0 ½ ½ , ½ 0 ½, ½ ½ 0.** So,



$$F = f\,[\,e^{2\pi i(0)} + e^{2\pi i(h/2+k/2)} + e^{2\pi i(k/2+l/2)} + e^{2\pi i(h/2+l/2)}\,]$$

$$= f\,[1 + e^{\pi i(h+k)} + e^{\pi i(k+l)} + e^{\pi i(h+l)}\,].$$

$F = 4f$, $|F|^2 = 16f^2$ when **all (hkl) are even/odd;**

$F = 0$, $|F|^2 = 0$ when **(hkl)** are **mixed.**

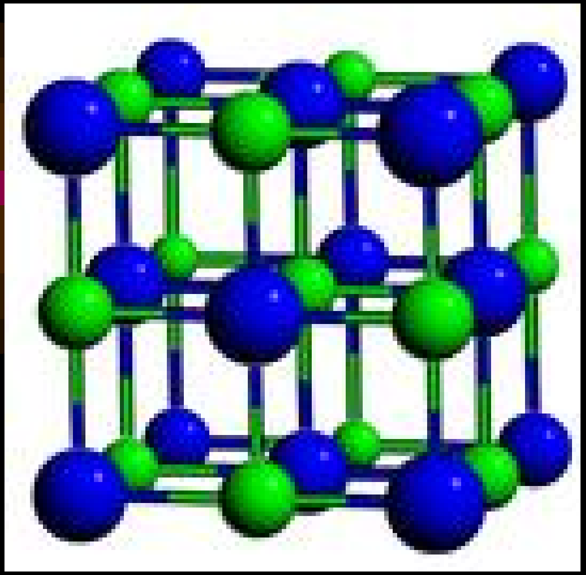
=> In the diffraction pattern ***no reflections occur*** for planes **(100), (210), (112),** etc. ***but reflections may occur*** for planes **(111), (200), and (220)** .

Example: NaCl

- Cubic lattice with 4 Na and 4 Cl atoms per unit cell, located at

Na 000, ½ ½ 0, ½ 0 ½, 0 ½ ½

Cl ½ ½ ½ , 0 0 ½ , 0 ½ 0, ½ 0 0



In this case, the proper atomic scattering factors for each atom must be used. So,

$$\begin{aligned}
F = f_{Na}\,[\, & e^{2\pi i(0)} + e^{2\pi i(h/2+k/2)} + e^{2\pi i(k/2+l/2)} \\
& + e^{2\pi i(h/2+l/2)}\,] \\
+ f_{Cl}\,[\, & e^{2\pi i(h/2+k/2+l/2)} + e^{2\pi i(l/2)} + e^{2\pi i(k/2)} \\
& + e^{2\pi i(h/2)}\,] \\
= [1 + & e^{\pi i(h+k)} + e^{\pi i(k+l)} + e^{\pi i(h+l)}\,] \\
& \times [f_{Na} + f_{Cl}\, e^{\pi i(h+k+l)}\,].
\end{aligned}$$

Note: The 1st term correspond to the face-centering translations and the 2nd factor contains the terms that describe the basis of the unit cell, namely the Na atom at 000 and Cl atom at ½ ½ ½ .

NaCl Structure Factor

$F = 0$, $|F|^2 = 0$ when **(hkl)** are **mixed.**

For unmixed indices,

$F = 4\,[f_{Na} + f_{Cl}\,e^{\pi i(h+k+l)}]$.

$F = 4(f_{Na} + f_{Cl})$ if **(h+k+l)** is **even;**

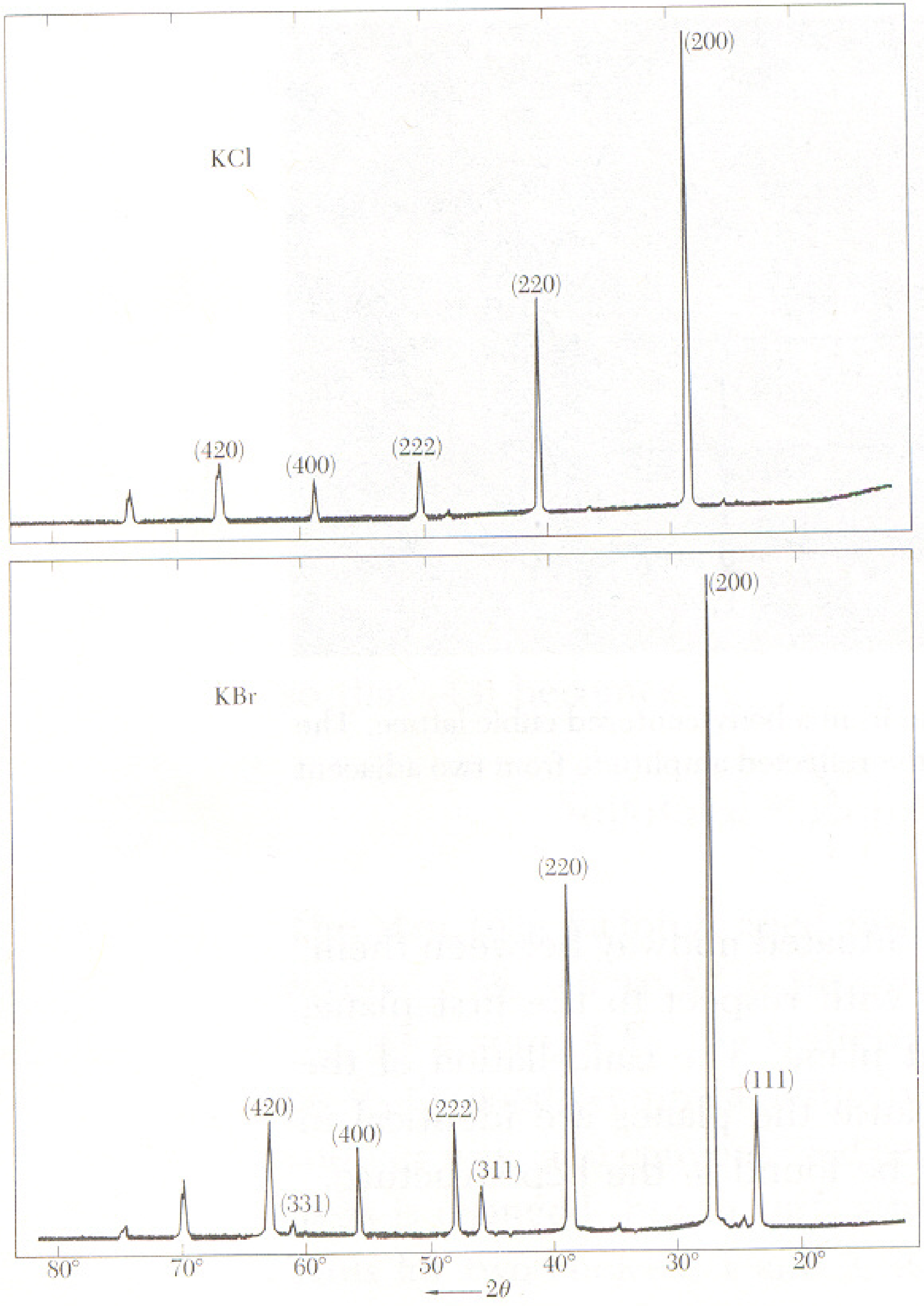
$|F|^2 = 16\,(f_{Na} + f_{Cl})^2$.

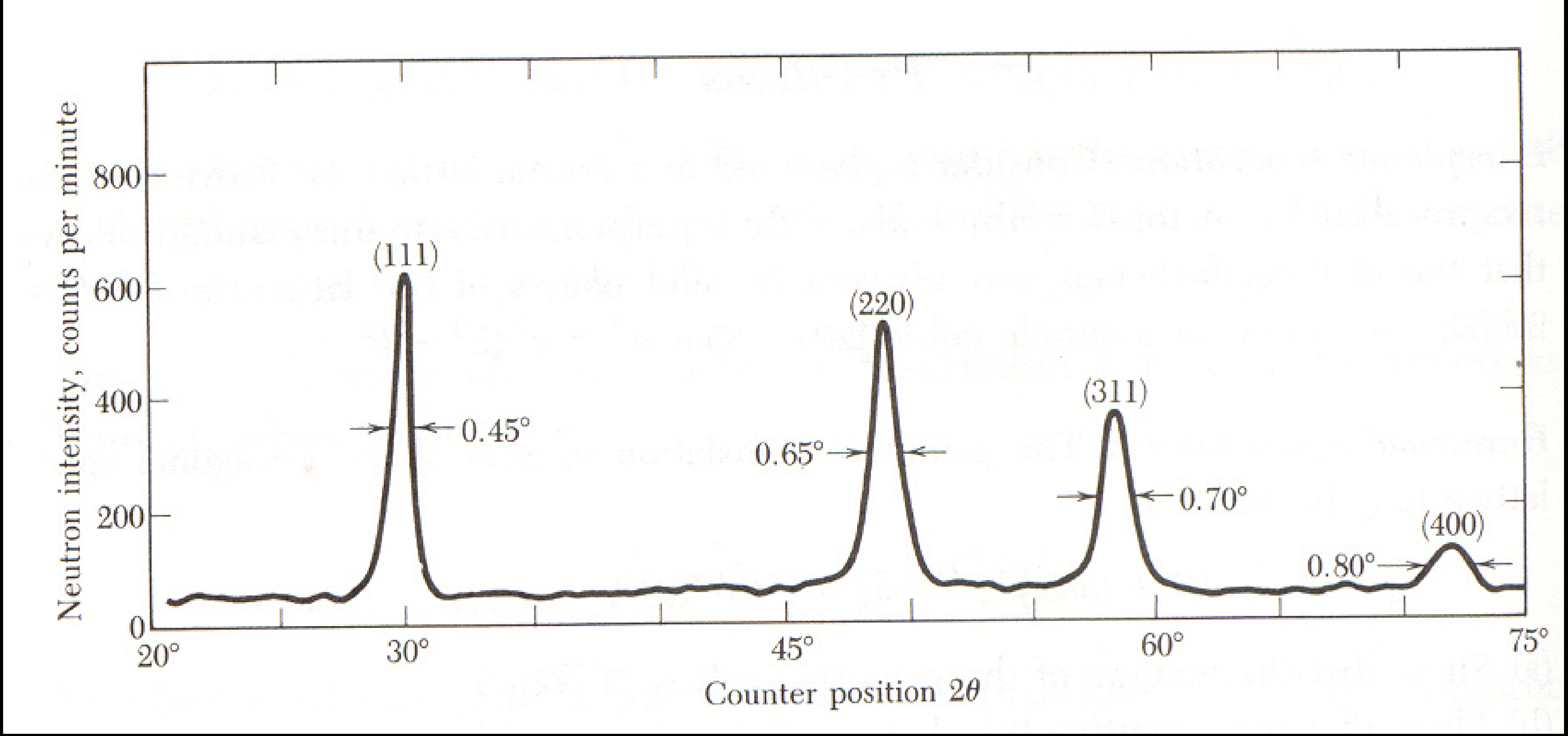
$F = 4(f_{Na} - f_{Cl})$ if **(h+k+l)** is **odd;**

$|F|^2 = 16\,(f_{Na} - f_{Cl})^2$.

X-ray reflections from KCl and KBr powders.

Both **KCl** and **KBr** have a FCC lattice, but **KCl** simulates a SC lattice with a lattice constant a/2 (Note: only even integer occur in the reflection indices) because the number of electrons of **K**$^+$ and **Cl**$^-$ ions are equal. So, the scattering amplitudes ***f*** **(K+)** and *f* **(Cl-)** are almost exactly equal. But in case of **KBr**, the form factor of **Br**$^-$ is quite different than that of **K+** , and all reflections of the FCC lattice are present.





Neutron diffraction pattern for powdered diamond.

The basis consists of eight atoms if the cell is taken as conventional cube. Allowed reflections of the diamond structure satisfy **$h+k+l = 4n$**, where ***all indices are even*** and **n** is any integer, or ***else all indices are odd***.

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Thanks to all of you!!