CRYSTALLOGRAPHY

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INTRODUCTION:

- Crystallography is the experimental science of determining the arrangement of atoms in crystalline solids.
- The word "crystallography" is derived from the Greek words crystallon "cold drop, frozen drop", with its meaning extending to all solids with some degree of transparency, and graphein "to write"

DISCOVERY:

- The field of **crystallography** started with the**discovery** of X-rays by Röntgen who was awarded the Nobel Prize in Physics for this**discovery** in 1901.
- Max von Laue followed this by investigating the interaction of X-rays with crystals producing a diffraction pattern and he received the Nobel Prize for Physics in 1914

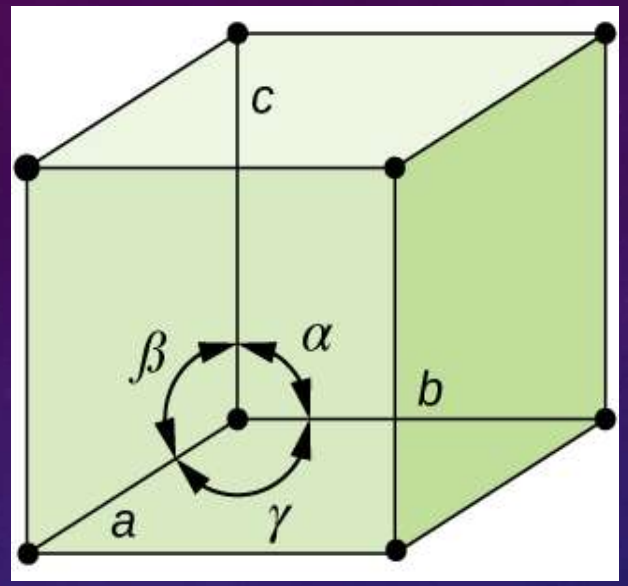
TYPES OF CRYSTAL:

There are in total 7 groups, collectively called**Crystal** Systems:

- Tricinic,
- Monoclinic,
- Orthorhombic,
- Tetragonal,
- Trigonal,
- Hexagonal, and
- Cubic.

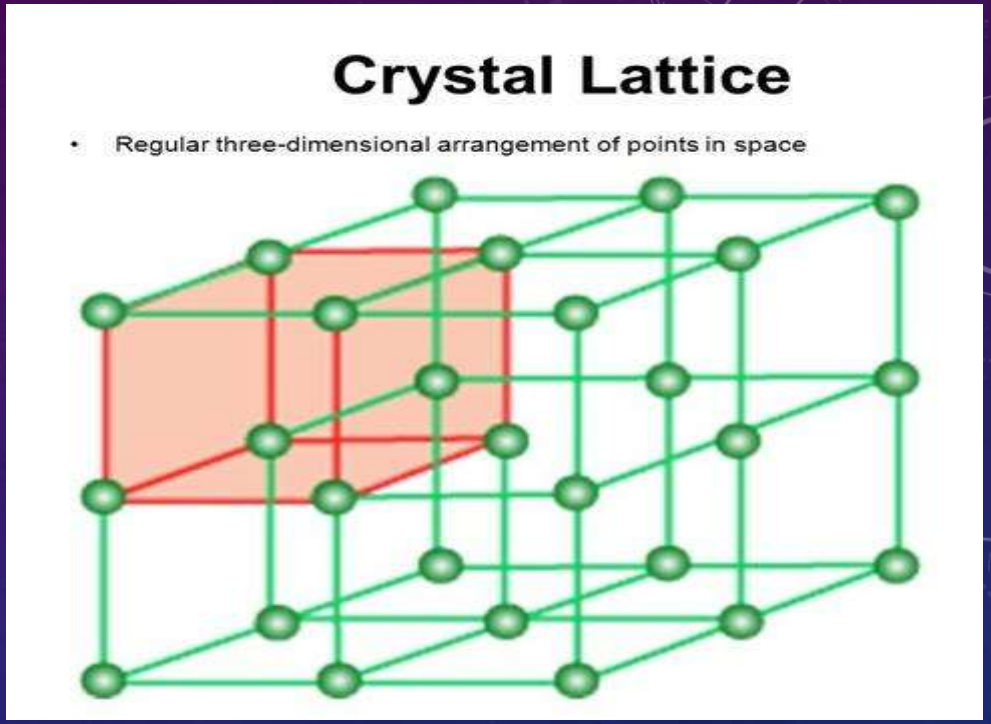
The symmetry of each group is described by the relationship between the lattice sides a, b, and c and angles α, β and γ.

UNIT CELL:



- The **unit cell** is defined as the smallest repeating **unit** having the full symmetry of the crystal structure.
- The geometry of the **unit cell** is defined as a parallelepiped, providing six lattice parameters taken as the lengths of the**cell** edges (a, b, c) and the angles between them (α, β, γ).

SPACE LATTICE:

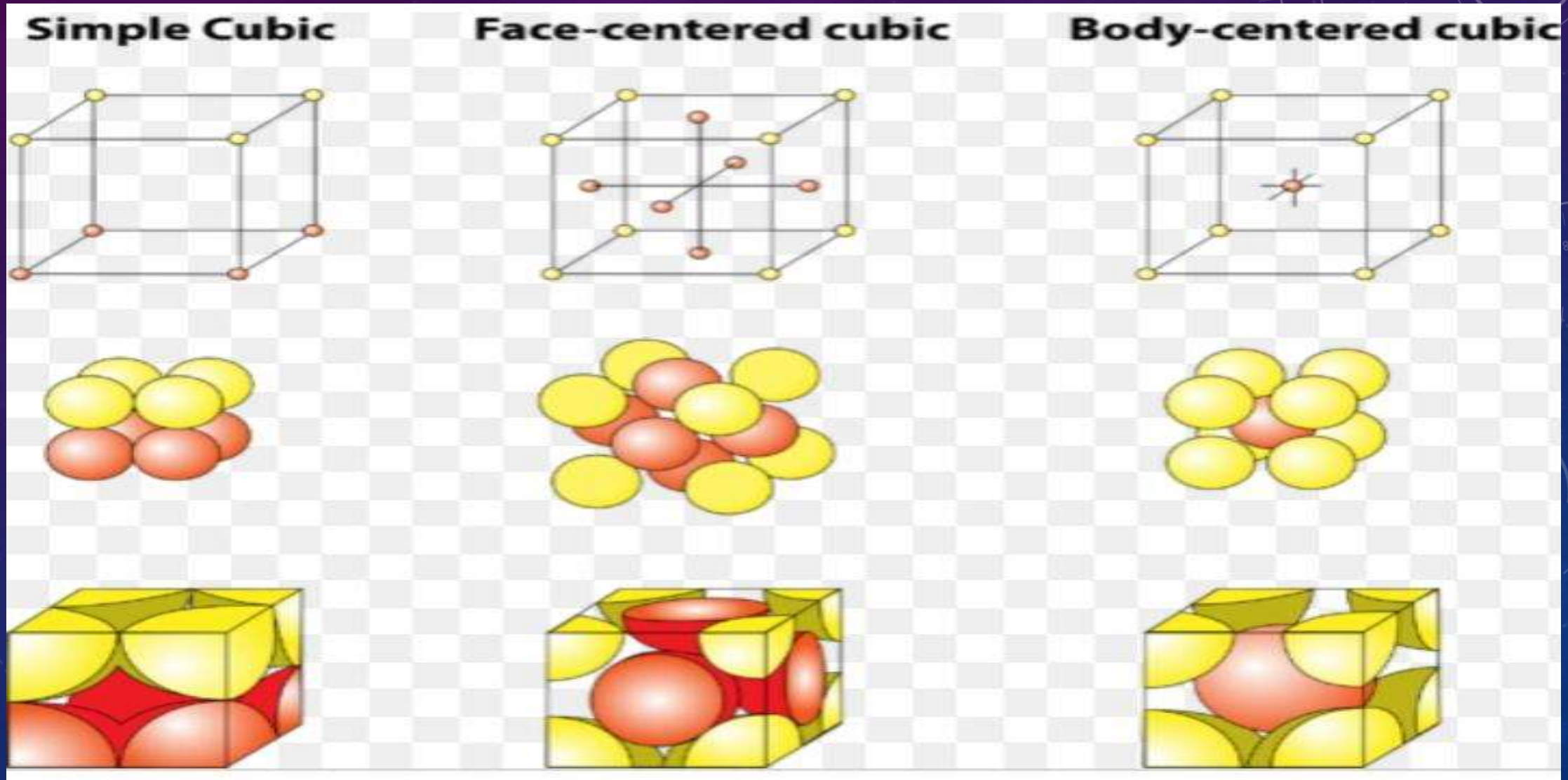


- A **space lattice** is an array of points showing how
- particles (atoms, ions or molecules) are arranged at different sites in three dimensional spaces

TYPES OF CUBIC CELLS:

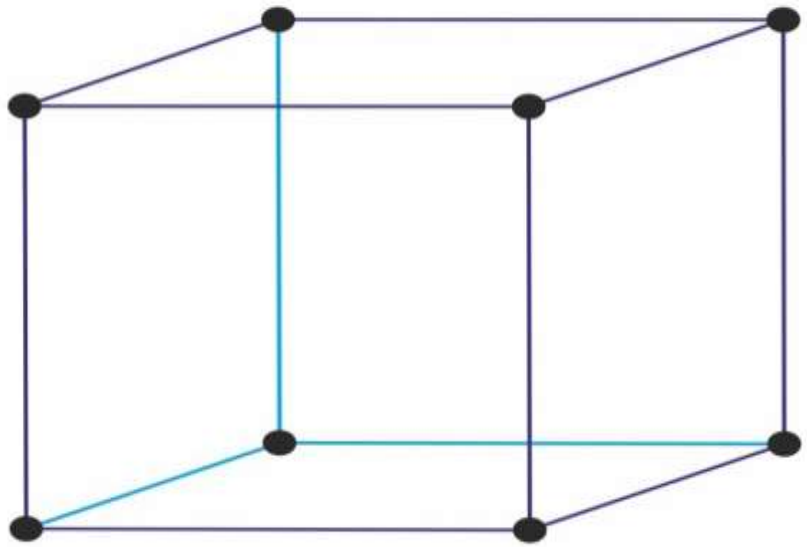
- **There are three main varieties of these crystals:**
- **Primitive cubic** (abbreviated cP and alternatively called simple cubic)
- **Body-centered cubic** (abbreviated cI or bcc)
- **Face-centered cubic** (abbreviated cF or fcc, and alternatively called cubic close-packed or ccp)

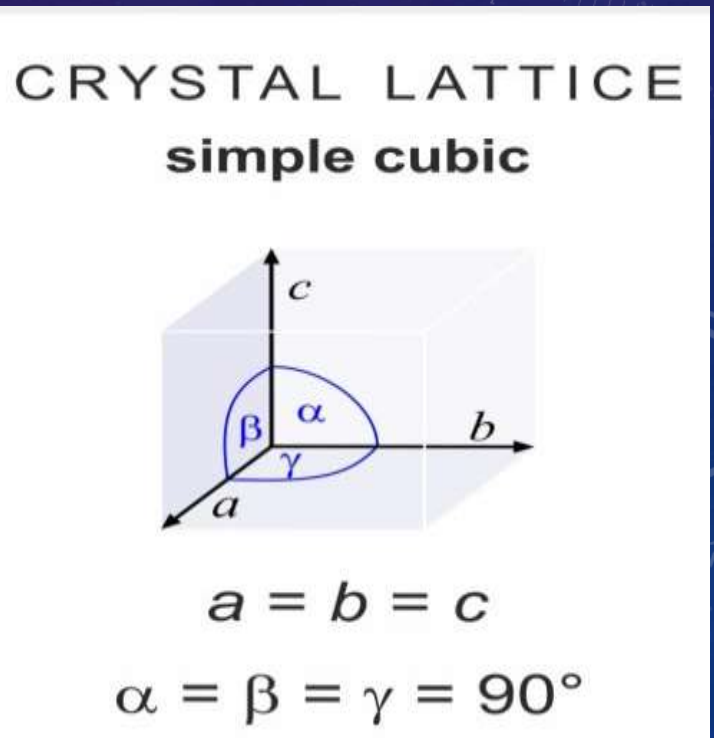
DIAGRAMATIC VIEW:



ARRANGEMENTS OF IDENTICAL SPHERES IN A SIMPLE CUBIC CELL:

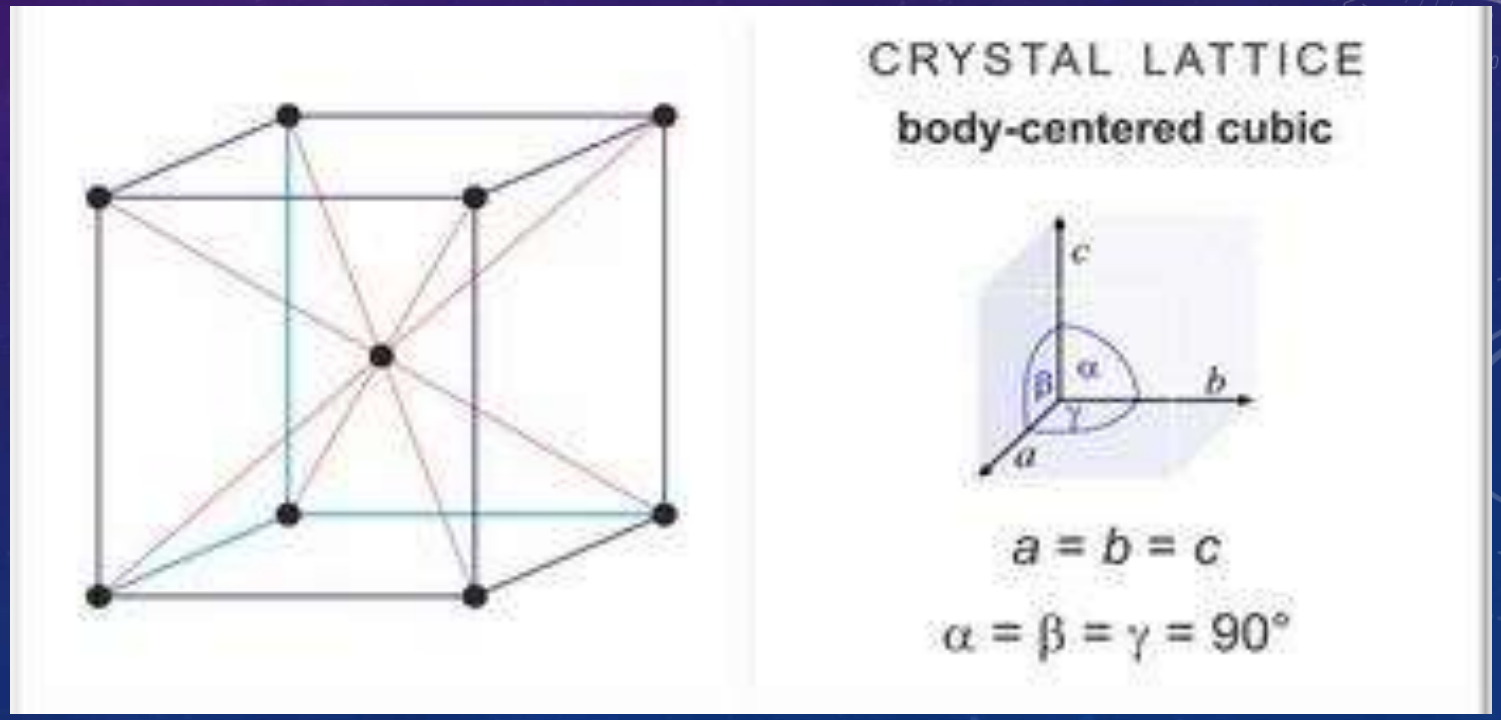
- Total no. Of atom per simple cubic cell is 8(1/8)= 1 atom





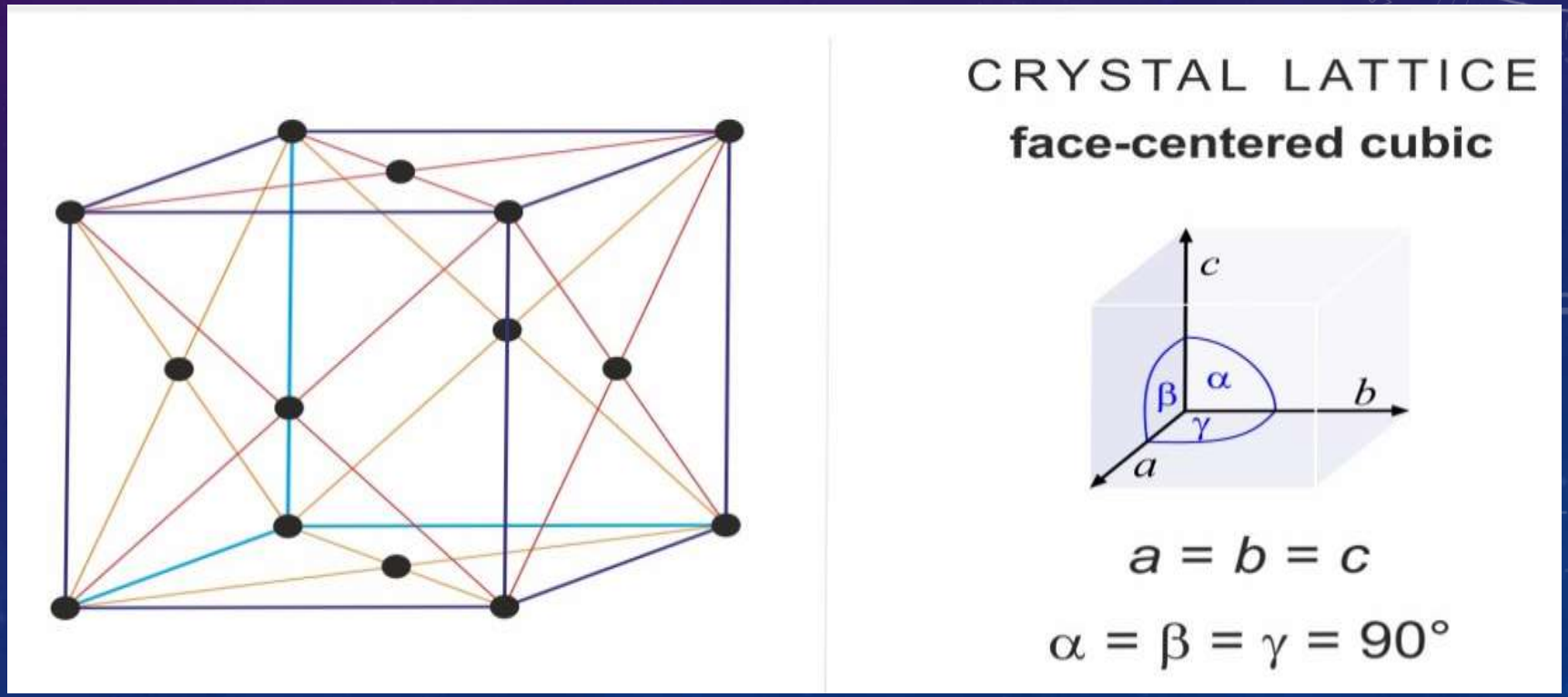
ARRANGEMENTS OF IDENTICAL SPHERES IN BODY CENTRED CUBE:

- Total no.of atom per BCC unit cell is 8(1/8)+1 =2 atoms

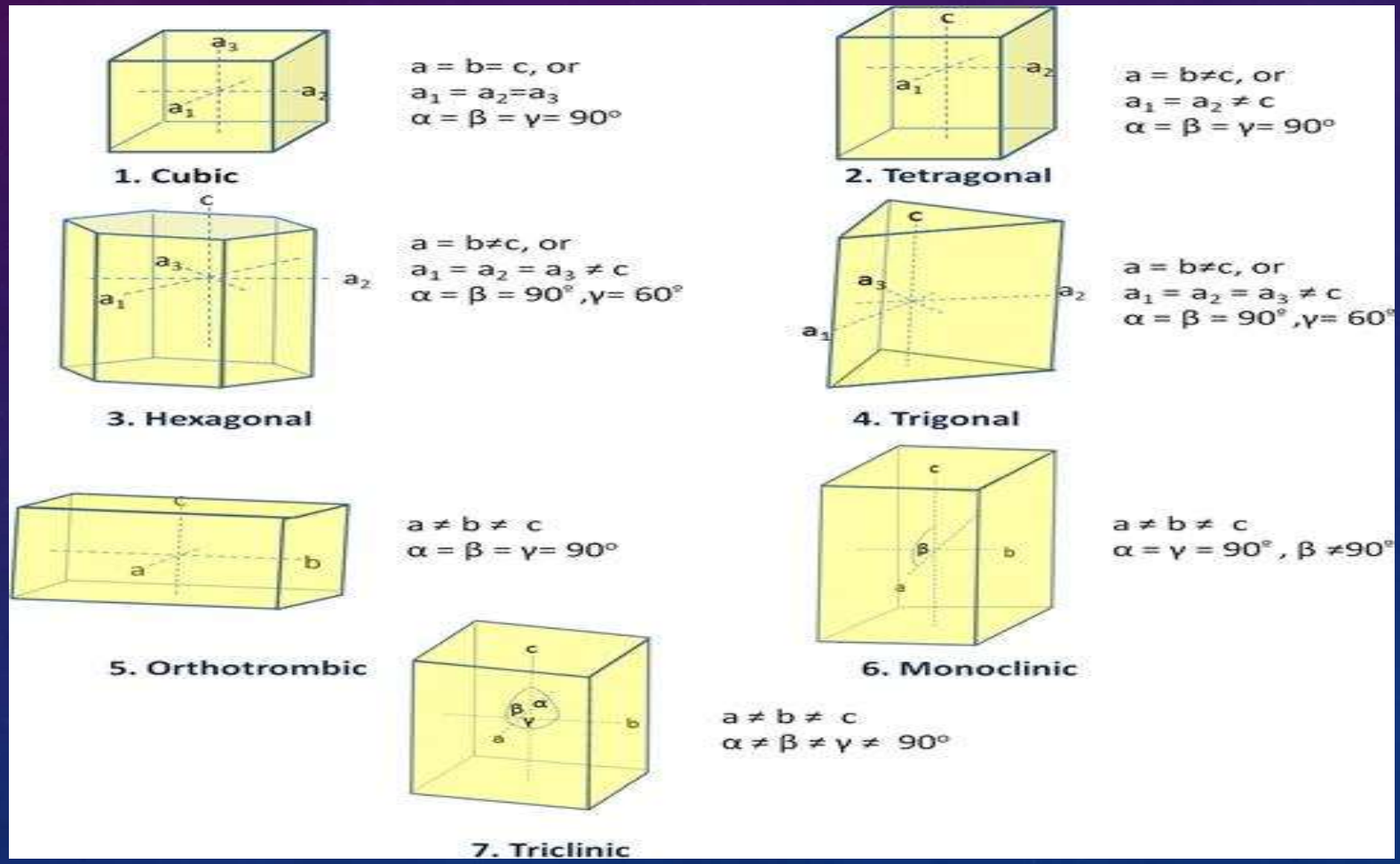


A CORNER ATOM AND A FACE CENTRED ATOM:

- Total no.of atom per FCC unit cell is 8(1/8)+6(1/2)= 4 atoms.



7 CRYSTAL SYSTEMS:



PRINCIPLE

- The underlying **principle** is that the crystalline atoms cause a beam of X-rays to diffract into many specific directions.
- By measuring the angles and intensities of these diffracted beams, a crystallographer can produce a 3D picture of the density of electrons within the crystal.

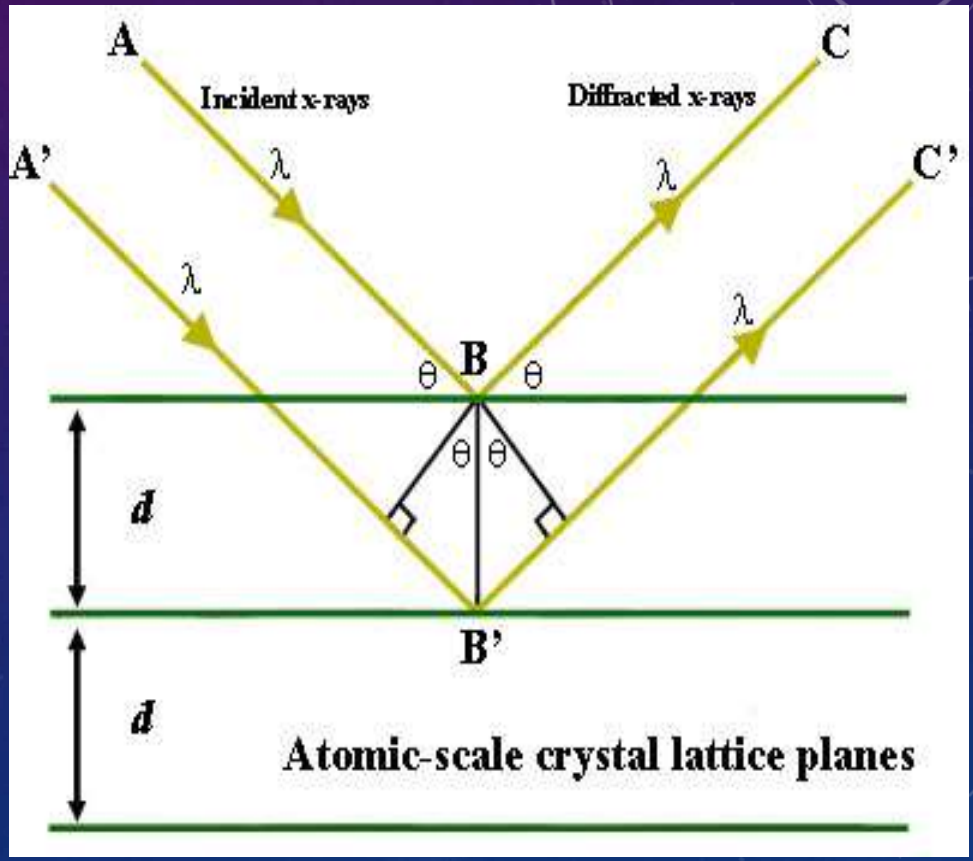
X RAY DIFFRACTION:

- a scattering of **X-rays** by the atoms of a crystal that produces an **interference effect** so that the **diffraction** pattern gives information on the **structure of the crystal** or the identity of a crystalline substance.
- Since **X-rays** have a **smaller wavelength than visible light,** they have higher energy and are more penetrative. Its ability to penetrate matter, however, is dependent on density of the matter. Therefore, **X-rays** are **useful** in exploring structures of atoms.

BRAGG'S LAW:

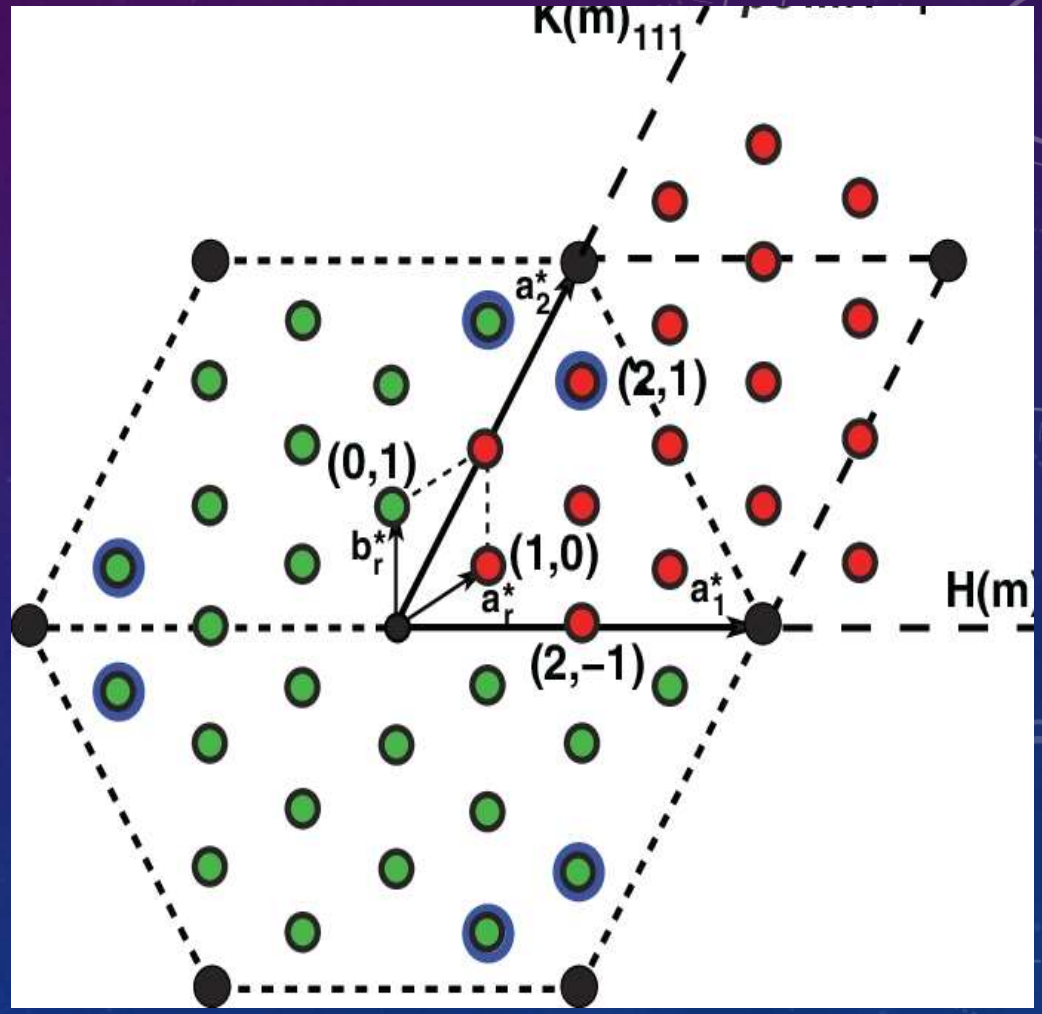
Bragg's law, or Wulff–**Bragg's** condition, a special case of Laue diffraction, gives the angles for coherent and incoherent scattering from a crystal lattice. When X-rays are incident on an atom, they make the electronic cloud move, as does any electrom.sgnetic wave.

- Braggg's equation : $n\lambda = 2d \sin\Theta$



RECIPROCAL LATTICE SPACE:

The **reciprocal space lattice** is a set of imaginary points constructed in such a way that the direction of a vector from one point to another coincides with the direction of a normal to the real **space** planes and the separation of those points (absolute value of the vector) is equal to the reciprocal of the real



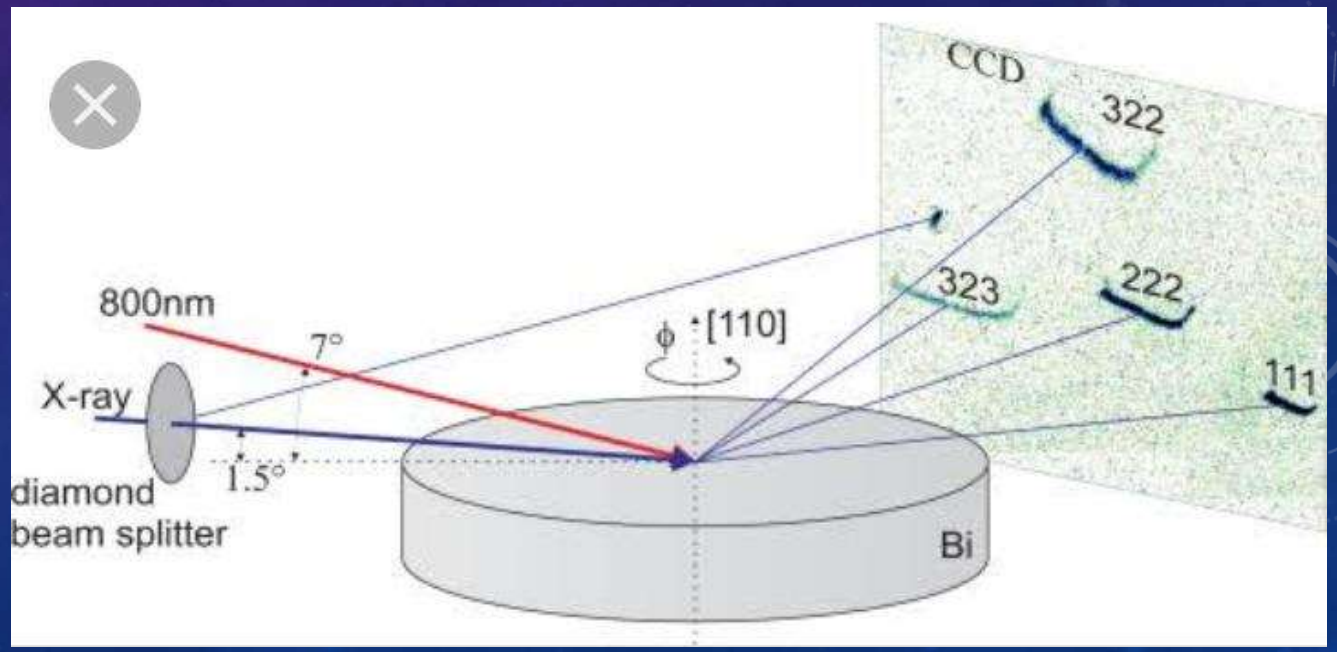
MILLER INDICES:

- any of a set of three numbers or letters used to indicate the position of a face or internal plane of a crystal and determined on the basis of the reciprocal of the intercept of the face or plane on the crystallographic axes.

ROTATING CRYSTAL METHOD:

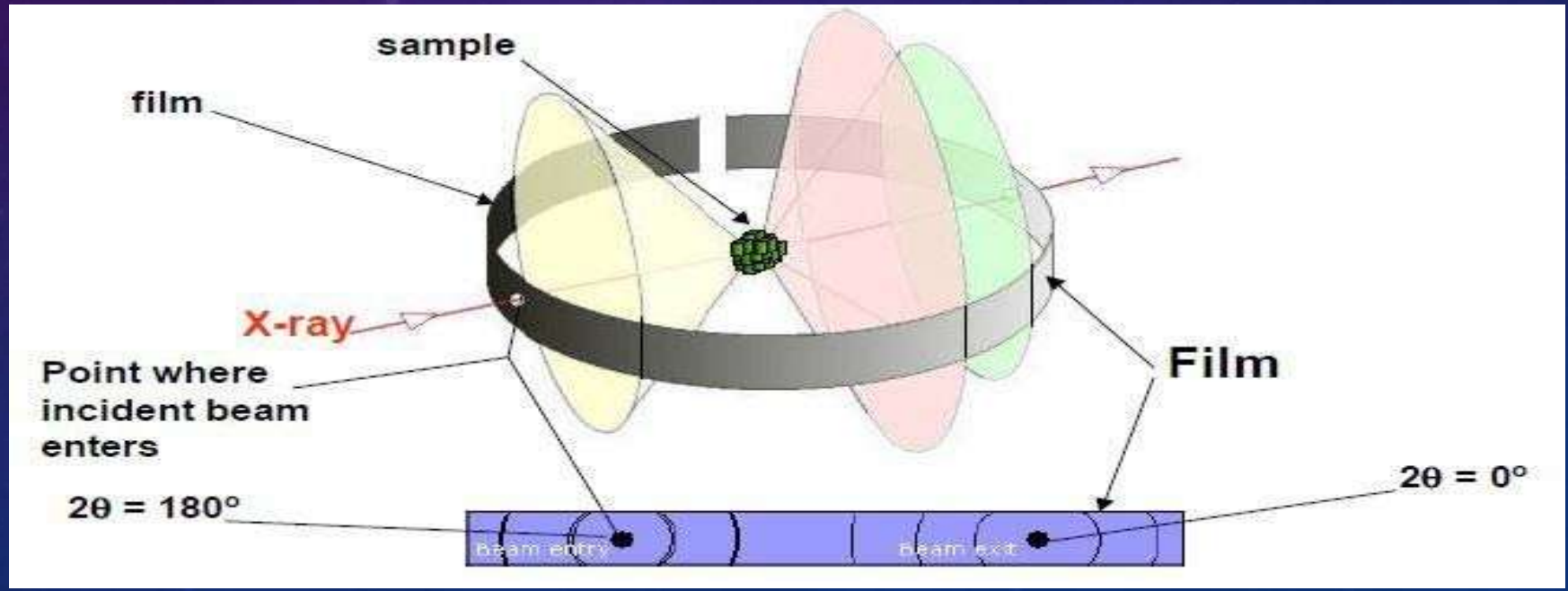
- The **rotation method** is the most common **method** to determine steady state **crystal** structures.

The orientation of the **rotation** axis and the **rotation** range can be chosen to select a subset of diffraction peaks fulfilling the Bragg condition $\Delta k = k - k = Hhkl(r,\phi)$.



POWDER METHOD:

- The **powder method** is used to determine the value of the lattice parameters accurately. ... A sample of some hundreds of crystals (i.e. a **powdered** sample) show that the diffracted beams form continuous cones. A circle of film is used to record the diffraction pattern as shown.




thank you