Crystallography Fundamentals

•Crystallography is the science that examines the arrangement of atoms in crystalline solids. Crystallography is a useful tool for materials scientists.

•Crystallography originated as the science of the study of macroscopic crystal forms, and the term “crystal” has been conventionally defined in terms of the structure and symmetry of these forms.

•The circumstances of a particular atom in a crystal has certain arrangement, and if one looks at the same kind of an atom at another place further along by the same distance, the conditions will be exactly the same.

• The arrangement is repeated over and over again and, of course, in three dimensions. This orderly arrangement in a crystalline material is known as the crystal structure.

•Modern crystallography is largely based on the analysis of the diffraction of X-rays by crystals acting as optical gratings. Using X-ray crystallography, chemists are able to determine the internal structures and bonding arrangements of minerals and molecules, including the structures of large complex molecules.

•Crystallographers use X-ray, neutron, and electron diffraction techniques to identify and characterize solid materials.

Crystal, Unit Cell, Space Lattice

A unit cell is the most basic and least volume consuming repeating structure of any solid. It is used to visually simplify the crystalline patterns solids arrange themselves in.

A space lattice is an array of points showing how particles (atoms, ions or molecules) are arranged at different sites in three dimensional spaces. Unit cells are easiest to visualize in two dimensions.

CHARACTERISTICS OF A CRYSTAL LATTICE - DEFINITION

1. In a crystal lattice there is the parallelepiped constructed from vectors which correspond to translational periods called unit cells.
2. These can be chosen in different ways. Commonly, unit cells are chosen so that its vertex coincides with one of the atoms of the crystal.
3. Then lattice sites are occupied by atoms, and of the atoms of the crystal.Thus, the lattice sites are occupied by atoms, and vectors that connect the nearest equivalent atoms.
4. The unit cell contains at least one atom of each of the types that make up the crystal.
5. Providing that the unit cell is made up of only one type of atom, it is called monatomic, anymore than that and it is polyatomic. Correspondingly a monatomic lattice is often identified as a simple lattice and a polyatomic one, a composite lattice.

Arrangement of atoms in cells

•A crystal is a regular, repeating arrangement of atoms. The simplest crystal conceptually is the so--called simple cubic structure, where the atoms lie on a grid: layers of rows and columns.

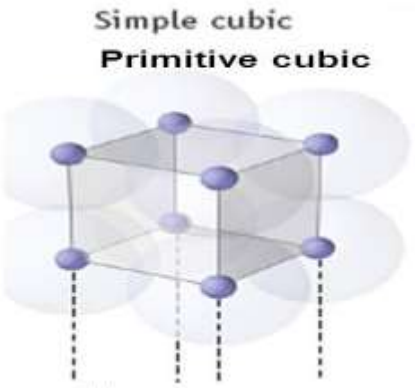
•A crystalline solid consists of repeating patterns of its components in three dimensions (a **crystal lattice**), we can represent the entire crystal by drawing the structure of the smallest identical units that, when stacked together, form the crystal.

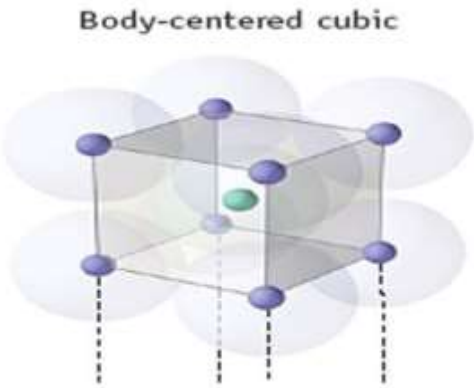
•This basic repeating unit is called a **unit cell**.

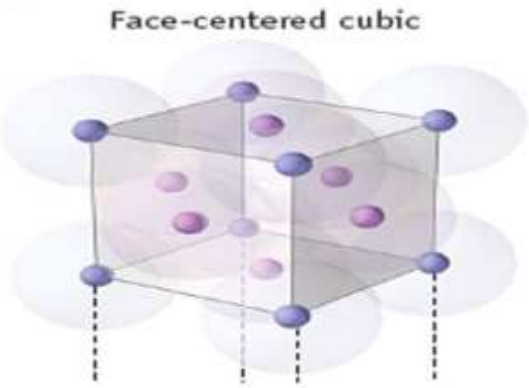
•If the cubic unit cell consists of eight component atoms, molecules, or ions located at the corners of the cube, then it is called **simple cubic.** If the unit cell also contains an identical component in the center of the cube, then it is **body-centered cubic (BCC).** If there are components in the center of each face in addition to those at the corners of the cube, then the unit cell is **face-centered cubic (FCC).**

•**Face centered cubic (FCC):** Atoms are arranged at the corners and center of each cube face of the cell.

•**Body-centered cubic (BCC).** Atoms are arranged at the corners of the cube with another atom at the cube center.







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