Basic of Crystallography
(Solid State Physics)

e-content for B.Sc Physics (Honours)
B.Sc Part-III
Paper-VII

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1. INTRODUCTION

- What is a Solid?
  - It is not a *continuous* rigid body, instead it is composed of discrete basic units (ATOMS).
  - Crystalline & Amorphous solids.

- Solid State Physics: Study of the properties of solid materials.
  - Mainly concerned with crystalline materials in this course.
  - Study of crystals triggered by discovery of X-ray diffraction by crystals.

- Why study solid state?
  - Integral part of physics
  - Important industrial applications, e.g. electronics, solid state devices, materials.

2. CRYSTALLINE STATE

- A *perfect crystal* maintains the periodicity of atoms from (∞) to ($-\infty$).
- Imperfections and the reality of the perfect crystal.

3. BASIC DEFINITIONS

The Lattice: is a geometrical pattern for the atomic arrangement in a crystal.

1. Bravais Lattice: all the lattice points (atomic sites) are *equivalent*.
2. Non-Bravais Lattice: some of the lattice points (atomic sites) are *not equivalent*.

Non-Bravais Lattice = Lattice + basis

The Basis: is a set of atoms located near each site of a Bravais lattice.

Basis Vectors: are a set of vectors in term of which the positions of all lattice points can be expressed.

The Unit Cell: In (2D), the area of the parallelogram whose sides are the basis vectors is called a *unit cell* of the lattice. There are two types of unit cells:

Primitive Unit Cell: which contains only one lattice point.

Nonprimitive Unit Cell: which contains more than one lattice point.

Useful Remarks:

* The same lattice may have more than one unit cell depending on the chosen basis vectors.

* All primitive unit cells – in this lattice- have the same area.

* The area of nonprimitive unit cell is an integral multiple of the primitive cell.

Non-Bravais Lattice $\neq$ Nonprimitive cell

In (3D)?

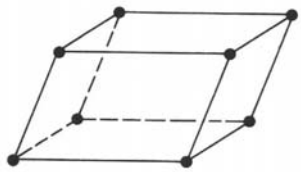
The same definitions BUT..

The lattice constant: (a) is the side length of the unit cell.

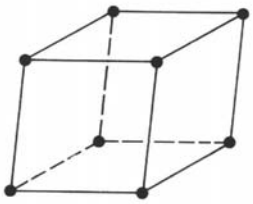
Co-ordination number: (z) is the number of nearest neighbours.

Packing fraction: ratio of the volume of atoms to available space in a unit cell.

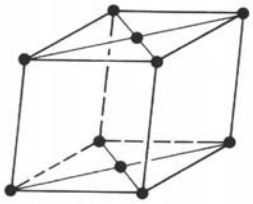
1. Bravais Lattices



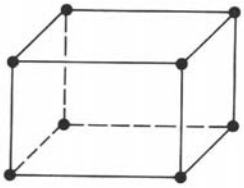
Triclinic



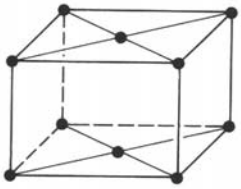
Simple monoclinic



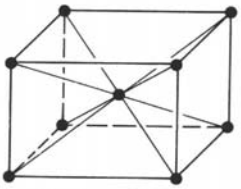
Base-centered monoclinic



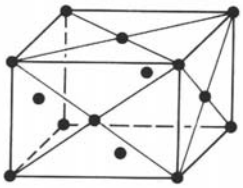
Simple orthorhombic



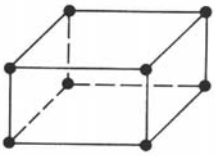
Base-centered orthorhombic



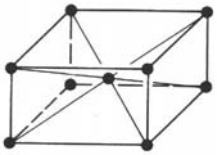
Body-centered orthorhombic



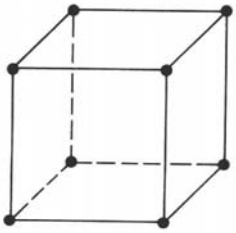
Face-centered orthorhombic



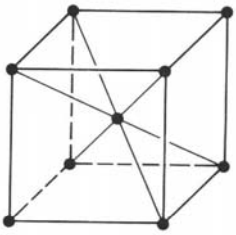
Simple tetragonal



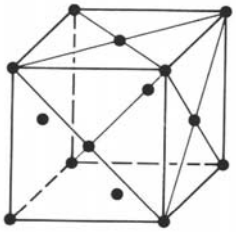
Body-centered tetragonal



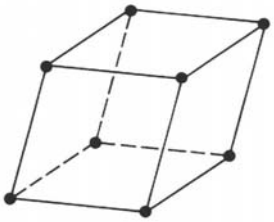
Simple cubic



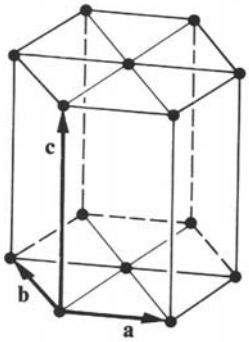
Body-centered cubic



Face-centered cubic



Trigonal



Hexagonal

Elements Of Symmetry:

Each of the unit cells of the fourteen lattices has one or more of the following elements of symmetry:

1. Inversion center: If there is a point at which transformation ($r \rightarrow -r$) can be preformed and the cell remains invariant.

FACT: All Bravais lattices are inversion symmetric.

2. Reflection plane: If a mirror reflection is performed on a plane and the cell remains invariant.

FACT: Not All Bravais lattices have a reflection plane

3. Rotation axis: If the cell rotated an angle (ϑ) around an axis and remains invariant. This axis is called n-fold axis of rotation

FACT: An angle $2\pi/n \Rightarrow n$-fold axis of rotation

2. Common Crystal Structures

2.1 Face Centered Cubic

- z = 12
- 4 atoms at 000, ½ ½ 0, ½ 0 ½ and 0 ½ ½.
- Examples: Cu, Au, Ag, Pb.
- Non-primitive unit cell.

2.2 Body Centered Cubic

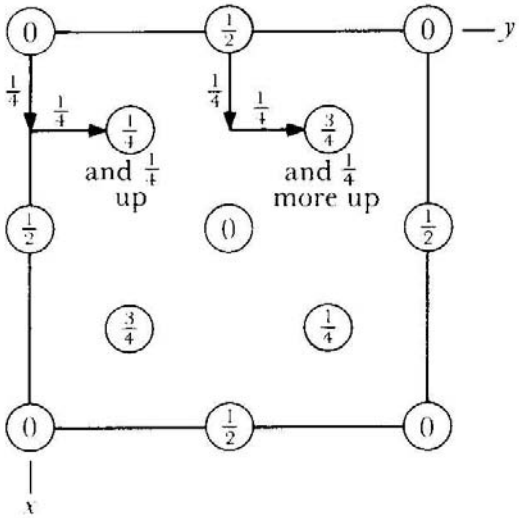
- z = 8.
- 2 atoms at 000 and ½ ½ ½ .
- Examples: Na, Li, K .
- Non-primitive unit cell.

Example1:

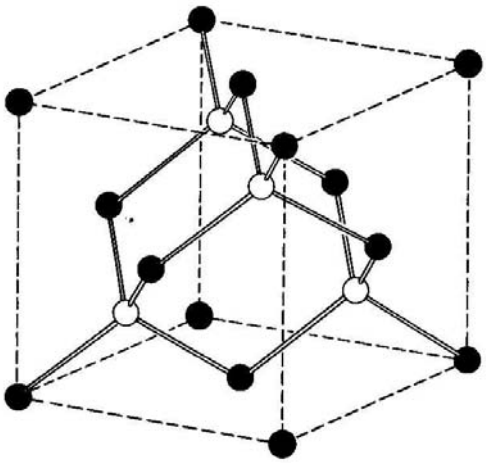
Calculate the packing fraction for an fcc structure.

2.3. Diamond & Related Structures

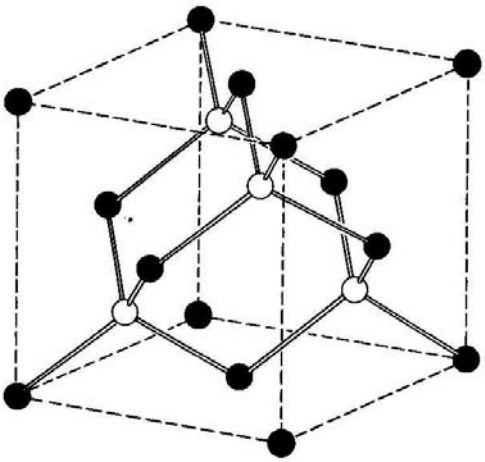
- The unit cell is an fcc cell with a basis of two atoms.
- z = 4.
- 8 atoms, where (group1) atoms located at 000, ½½0, ½0½, 0½½ , and (group2) atoms located at ¼¼¼, ¼¾¾, ¾¼¾, ¾¾¼.



- Examples:



(group 1) & (group 2) same
⇒ Diamond Structure:
C, Si, Ge



(group 1) & (group 2) different
⇒ Zincblende Structure:
GaAs, ZnS, InSb.

2.4. Ionic Structures

1. NaCl structure:

Non-Bravais lattice composed of two fcc sublattices displaced relative to each other by ½**a**.

One made up of 4 Na atoms (at 000, ½½0, ½0½, 0½½;) and the other of 4 Cl atoms (at ½00, 0½0, 00½, ½½½).

- $z = 6$.

2. CsCl structure:

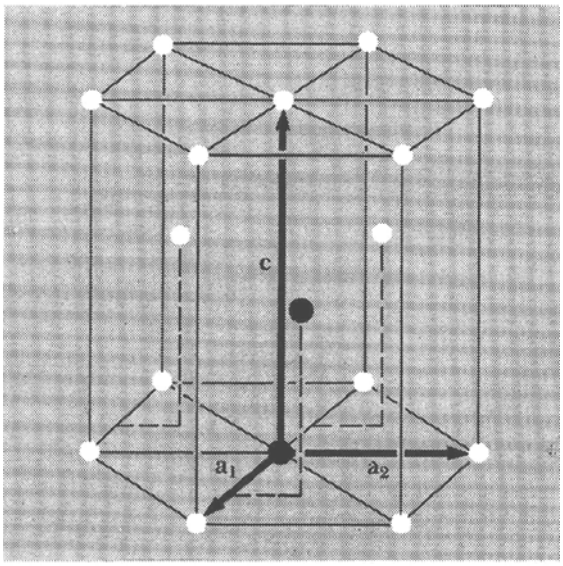
Non-Bravais lattice composed of two sc sublattices displaced relative to each other by $\frac{\sqrt{3}}{2}$ **a**.

One made up of 1 Cs atom (at 000) and the other of 1 Cl atom (at ½½½).

- $z = 8$.

2.5 Hexagonal close-packed *hcp* Structure

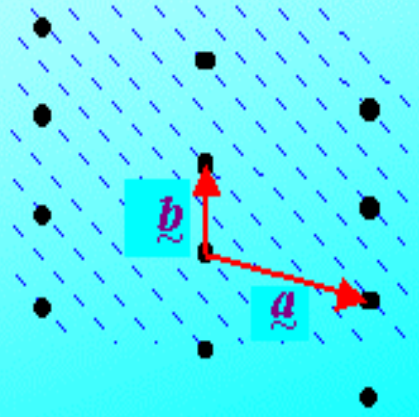
- The unit cell is a simple hexagonal cell with a basis of two atoms one at (000) and the other at (2/3 1/3 1/2) .
- z = 12.
- 6 atoms per unit cell.
- The ratio c/a =1.633.



3. Crystal Planes & Directions

- What are the lattice planes? sets of equally spaced *parallel* planes within lattice.
  - Each plane of a set has the same density of lattice points.
  - All lattice points are contained on each set of planes.
  - Lattice planes important in crystal diffraction experiments.
- Miller Indices (*hkl*): Derived from the intercepts made on the crystal axes by the plane that is nearest to the origin.

Intercepts at $a/3$ and $b/2$.
Miller Indices for plane is: (3 2)
—Large indices indicate closer planes.
Exercise: Which plane does (1 0) represent?



To determine the indices for a plane:

- Find its intercepts with the axes.
- Take their reciprocals.
- Reduce them to the smallest integers by multiplying by a common factor.
- Write the set into round brackets ().

To determine a direction:

- Find the components of a vector in that direction.
- Reduce them to the smallest integers.
- Write them into square brackets [].

Convention:

- General plane: (*h k l*)
- Negative intercept represented by bar above number.
- Directions are conventionally represented with square brackets, eg. [2 1 2], while Planes are represented with round brackets, eg. (2 1 2).