Unit: Solid State

B.Sc-I

Paper-1

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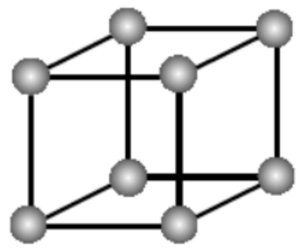
Number of Atoms in a Unit Cell

We know that a crystal lattice comprises of several unit cells. In a unit cell, every constituent particle (atom, molecule or ion) has a specific and fixed position called lattice site. We can calculate a number of atoms/molecules and ions in a unit cell easily by analyzing the nature and position of constituent particles in unit cells.

1. **Primitive Cubic Unit Cell**



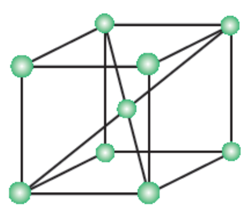
In the primitive cubic unit cell, the atoms are only located on the corners. That means 8 atoms are located on 8 corners of the lattice. Each atom located on the corner contributes 1/8th of the original volume of the cell. Since there are total 8 atoms in a primitive cubic unit cell,

Therefore total number of atoms in the primitive cubic unit cell = $8\times\frac{1}{8} = 1$

So there is only 1 atom in a primitive cubic unit cell.

2. **Body-Centred Unit Cell**

A body-centred cubic (*bcc*) unit cell has an atom at each of its corners and also one atom at its body centre.



Thus in a body-centered cubic (bcc) unit cell:

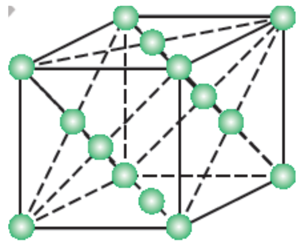
(i) 8 corners ×1⁄8 per corner atom = 8×1/8 = 1 atom

(ii) 1 body centre atom = 1 × 1 = 1 atom

Therefore Total number of atoms per unit cell = 1+1 = 2 atoms

3. **Face-Centred Unit Cell**

A face-centred cubic (*fcc*) unit cell contains atoms at all the corners and at the centre of all the faces of the cube. It is clear from the figure that each atom located at the face-centre is shared between two adjacent unit cells and only 1/2 of each atom belongs to a unit cell.



Thus, in a face-centred cubic (*fcc*) unit cell:

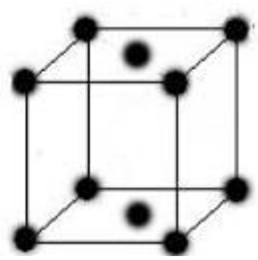
(i) 8 corners atoms ×1/8 atom per unit cell = 8× 1/8 = 1 atom

(ii) 6 face-centred atoms ×1/2 atom per unit cell = 6 × 1/2 = 3 atoms

Therefore total number of atoms per unit cell = 1 + 3 = 4 atoms

4. End-Centred Unit Cell

In end-centred cubic unit cell, 8 atoms are located on 8 corners of the cube and 1 atom each is present on two opposite faces of the cube.



Thus, in a end-centred cubic unit cell:

(i) 8 corners atoms ×1/8 atom per unit cell = 8× 1/8 = 1 atom

(ii) 2 opposite face-centred atoms ×1/2 atom per unit cell = 2 × 1/2 = 1 atoms

Therefore total number of atoms per unit cell = 1 + 1 = 2 atoms