Backup Question 1:

Calculate the following parameters for Al (FCC, a=4.05):

The number of atoms per unit cell.

The nearest neighbor distance.

The atomic radius *r*.

The surface density.

The volume density of atoms in the crystal.

The packing factor of the crystal.

Solution 1:

1. Number of Atoms per Unit Cell:

Number of atoms per unit cell = 8 *1/8 + 6*1/2 = 1 + 3 = 4

2. Nearest Neighbour Distance:

In an FCC structure, the nearest neighbours are located along the face diagonals. The face diagonal can be calculated as:

The nearest neighbor distance dnn is half of the face diagonal:

Nearest Neighbour Distance, dnn = = 2.86 A

3. Atomic Radius, r:

r = dnn/2 = 2.86/2 Å = 1.43 Å

4. Surface Density on the (100) Plane:

Number of atoms per surface = 1+4*1/4 = 2

Area = a^2 = 4.05^2 = 16.4 A^2

Surface Density = Number of atoms on the plane/Area of the plane = 2/16.4 = 0.122 atoms/Å^2

5. Volume Density:

Volume Density = Number of atoms in the unit cell/Volume of the unit cell= 4/a^3 = 4/4.05^3

= 4/6.64*10^(-23) = 6.02 * 10^(22) atoms/cm^3

6. Packing Factor:

Packing Factor = Volume occupied by atoms in the unit cell/Volume of the unit cell

Volume occupied by the atoms in the unit cell = 4 *

Packing Factor = 0.735

Backup Question 2:

Calculate the following parameters for W (BCC, a=3.165):

The number of atoms per unit cell.

The nearest neighbor distance.

The atomic radius *r*.

The surface density.

The volume density of atoms in the crystal.

The packing factor of the crystal.

Solution 1:

1. Number of Atoms per Unit Cell:

Number of atoms per unit cell = 8 *1/8 + 1 = 2

2. Nearest Neighbour Distance:

In an FCC structure, the nearest neighbours are located along the face diagonals. The face diagonal can be calculated as:

The nearest neighbor distance dnn is half of the face diagonal:

Nearest Neighbour Distance, dnn = = 2.74 A

3. Atomic Radius, r:

r = = = 1.58 Å

4. Surface Density on the (100) Plane:

Number of atoms per surface = 4*1/4 = 1

Area = a^2 = 3.165^2 = 10.02 A^2

Surface Density = Number of atoms on the plane/Area of the plane = 1/10.02 = 0.1 atoms/Å^2

5. Volume Density:

Volume Density = Number of atoms in the unit cell/Volume of the unit cell= 2/a^3 = 2/3.165^3

= 2/3.17*10^(-23) cm^3 = 6.31 * 10^(22) atoms/cm^3

6. Packing Factor:

Packing Factor = Volume occupied by atoms in the unit cell/Volume of the unit cell

Volume occupied by the atoms in the unit cell = 2 *

Packing Factor = 0.524