

Introduction to Solid State Physics (BSc-III)

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Primitive Cells in Cubic System

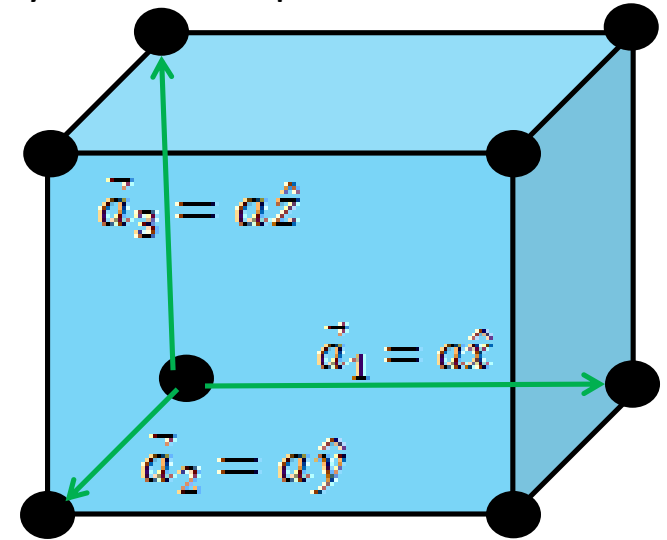
Primitive cells are those cells which contain only one lattice point.

Simple Cubic lattice

Since the conventional lattice of simple cubic lattice contains only one lattice Point per unit cell so the conventional lattice is the Primitive cell.

The primitive vectors are given as

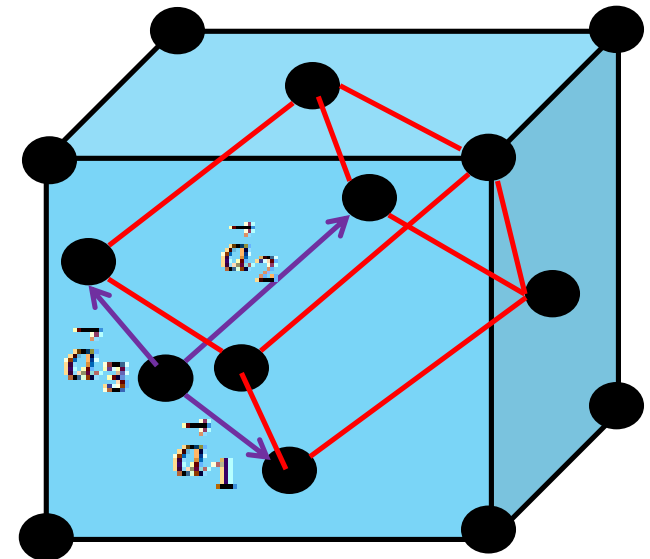
$$\vec{a}_1 = a\hat{x} \quad \vec{a}_2 = a\hat{y} \quad \vec{a}_3 = a\hat{z}$$



Face centered cubic lattice

Conventional cell is FCC but its primitive Cell is a rhombohedron made with 2 corner atom and all the atoms at the face center. The primitive vectors are Given as

$$\vec{a}_1 = \frac{1}{2}(\hat{x} + \hat{y}) \quad \vec{a}_2 = \frac{1}{2}(\hat{y} + \hat{z}) \quad \vec{a}_3 = \frac{1}{2}(\hat{z} + \hat{x})$$



Body centered cubic lattice

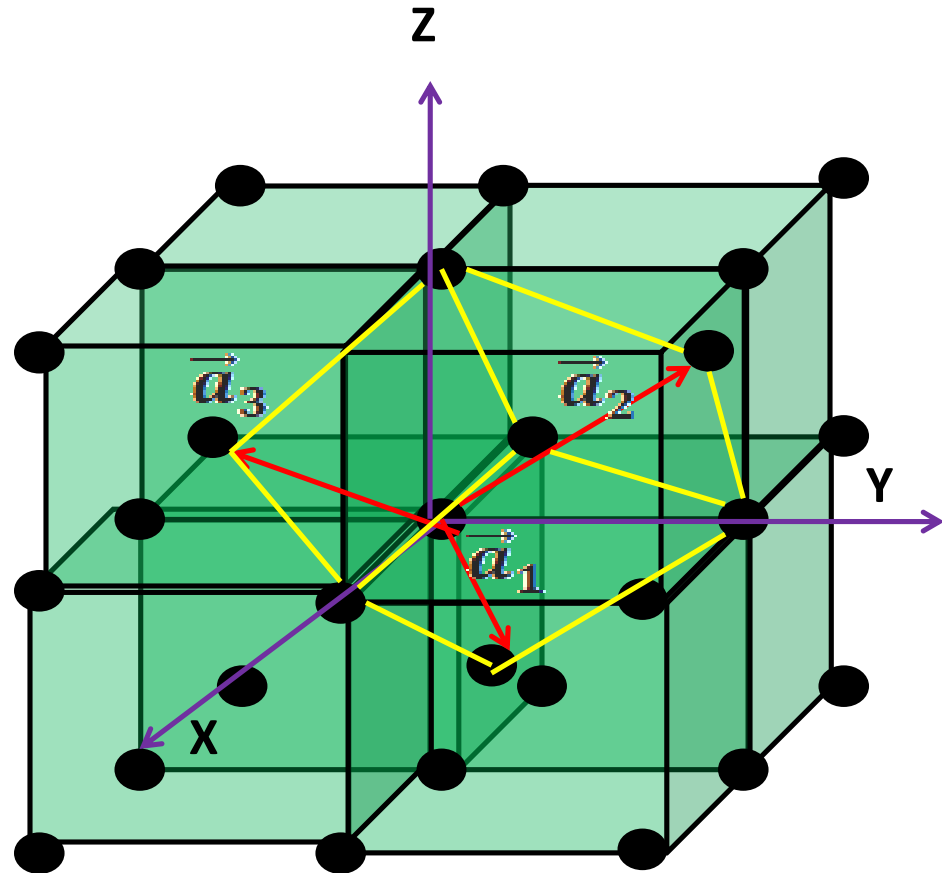
The atoms are at the corners and the body center. The primitive unit cell of bcc lattice is a rhombohedral and it is made by joining the three primitive vectors of bcc lattice. The primitive vectors are given as

$$\vec{a}_1 = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z})$$

$$\vec{a}_2 = \frac{a}{2}(-\hat{x} + \hat{y} + \hat{z})$$

$$\vec{a}_3 = \frac{a}{2}(\hat{x} - \hat{y} + \hat{z})$$

The primitive lattice is shown
By yellow lines.

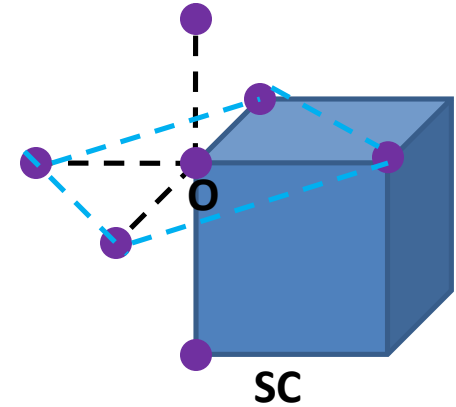


Coordination number

Coordination number is the number of nearest neighbors in a crystal system

Simple Cubic

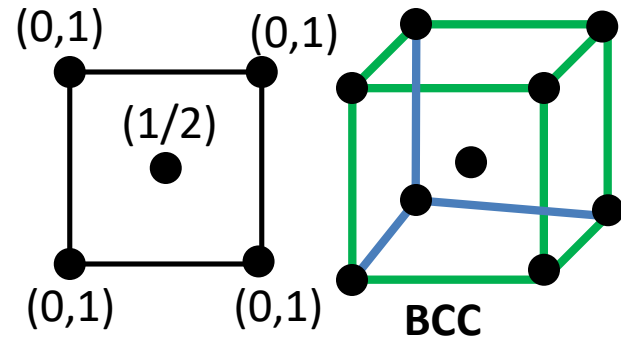
Here we can see that the atom at O is connected to 4 Other atoms in the same plane while two other atoms Are connected to it along vertical axis
So coordination number in simple cubic system is 6
Each along positive axes and each along negative Axes.



BCC

Here eight corner atoms are at same distance from the atom at the body centre.

So the coordination number of the atom at the body centre is 8 while the Coordination number of the atoms at any of the corners is also 8 as there will be one body centered atom in each and every unit cell around the selected corner atom.



FCC

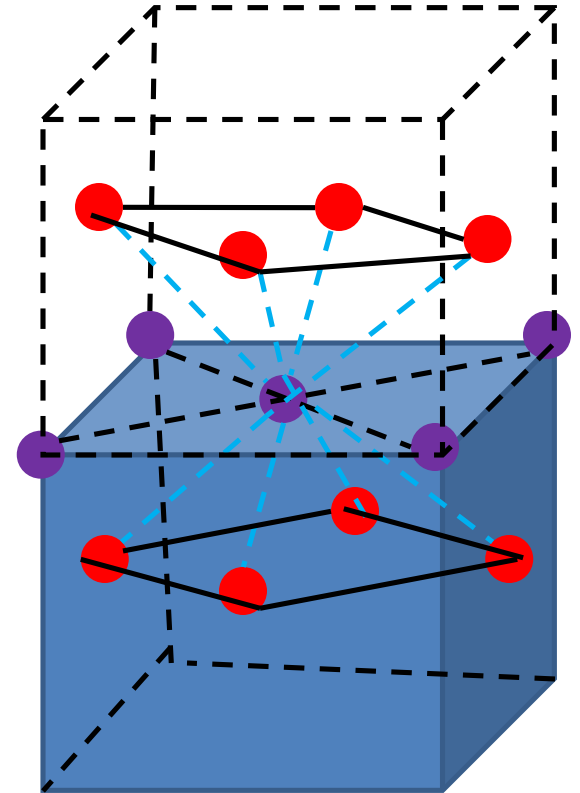
Here we can see that for an atom on the face centre
We have four corner atoms, 4 atoms on the faces of
Unit Cell above this cell and 4 other face centered
atoms below this unit cell.

$$\begin{aligned} \text{So coordination number of a} \\ \text{face centered atom} &= 4 + 4 + 4 \\ &= 12 \end{aligned}$$

Similarly considering a corner atom we have 6
other atoms along the cube edges and 6 other
atoms at the nearest face centers

$$\begin{aligned} &= 6 + 6 \\ &= 12 \end{aligned}$$

So CN=12 in FCC



Packing Fraction

The packing fraction is defined as the ratio of volume occupied by the atoms in a unit cell to the volume of the Unit cell

$$\text{Packing fraction} = v/V$$

Where, v = volume of the atoms and V = volume of the unit cell

Simple Cubic Structure

Here in a simple cubic system all the corner atoms touch its nearest corner atoms

$$\text{So } a=2r$$

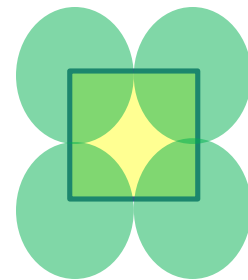
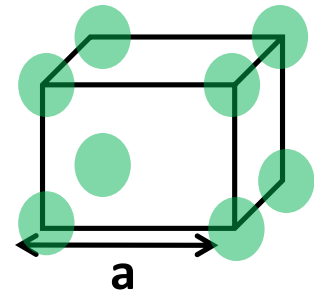
$$P F = \frac{1 \cdot \frac{4\pi r^3}{3}}{a^3}$$

Putting $r=a/2$,

$$P F = \frac{\pi}{6}$$

Or

$$P F = 52\%$$



Body Centered Cubic Structures

In a BCC structure the atoms are at the corners and one at the body center of unit cell. Here we have shown the two dimensional view of a BCC structure.

Here atoms at the corners touch the Atom at the body centre so

$$4r = a\sqrt{3}$$

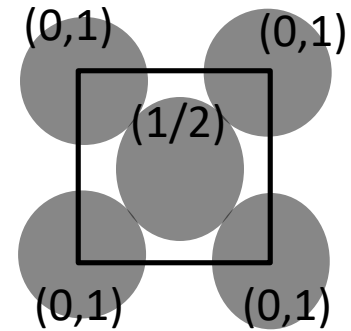
$$a = (4r/\sqrt{3})$$

Since the number of atoms in a BCC structure is 2, the packing fraction will be given by

$$P F = \frac{2 \cdot \frac{4\pi r^3}{3}}{a^3}$$

Putting, $a = 4r/\sqrt{3}$, we get $P F = \frac{\pi\sqrt{3}}{8}$

Or P. F. = 68%



Face Centered Cubic Structures

The atoms in FCC structures are present at the corners of the cube and also at the face diagonals. The atoms at a face diagonal touch the atoms at the corners.

$$\text{So } 4r = a\sqrt{2}$$

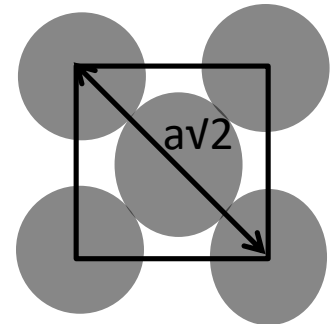
Since total number of atoms in a FCC Structure is 4, So the Packing Fraction is given by

$$P F = \frac{4 \cdot \frac{4\pi r^3}{3}}{a^3}$$

Putting $r = a/(2\sqrt{2})$, we get

$$P F = \frac{\pi}{3\sqrt{2}}$$

$$P. F. = 74\%$$



Different examples of Simple Cubic(SC), Body Centered Cubic(BCC) and Face Centered Cubic(FCC) Structures

Simple Cubic structure

CsCl is an example of Simple cubic lattice

Here all the Cs atoms are at the corners of the cube

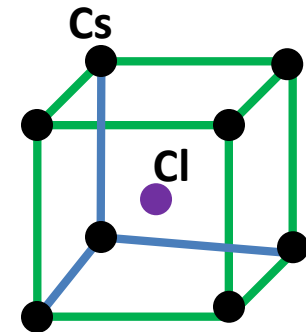
So $8 \times \frac{1}{8} = 1$ Cs atom per unit Cell

(Since corners contribute only $\frac{1}{8}$ part of an atom)

And one Cl atom at the body centre of the cube

So total one CsCl molecule in the unit cell at the lattice point

Here $a=b=c=4.11\text{\AA}$



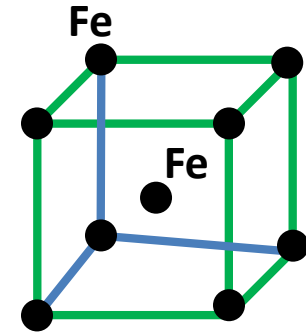
Body Centered Cubic structure

α -iron has BCC lattice

Here all the atoms sitting at corners are contributing

$$8 \times \frac{1}{8} = 1 \text{ atom}$$

And one iron atom sits at the body centre of the cube



So $1+1=2$ atoms/unit cell

Here $a=b=c=2.86 \text{ \AA}$

Face Centered Cubic structure

NaCl has FCC lattice

$$a=b=c=5.63 \text{ \AA}$$

Atomic positions in an unit cell is given as following

Na > $(0, 0, 0), (\frac{1}{2}, \frac{1}{2}, 0), (\frac{1}{2}, 0, \frac{1}{2}), (0, \frac{1}{2}, \frac{1}{2})$

Cl > $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}), (0, 0, \frac{1}{2}), (0, \frac{1}{2}, 0), (\frac{1}{2}, 0, 0)$

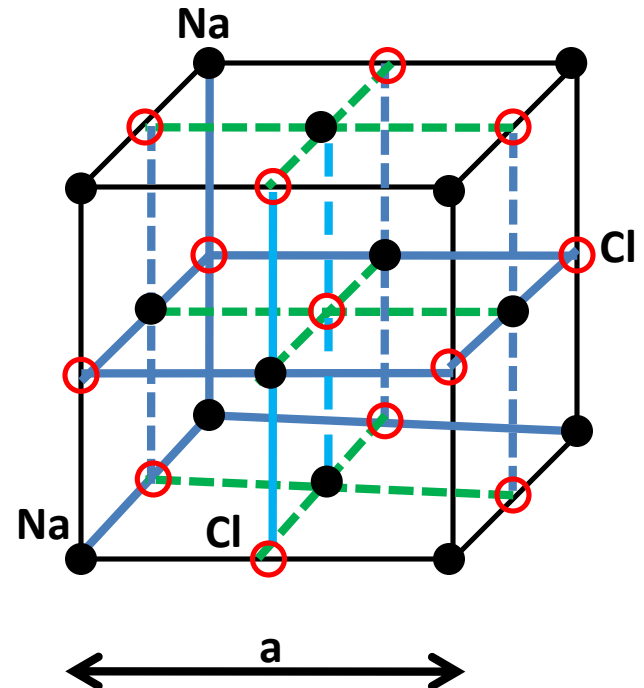
Therefore the total number of atoms of one kind in FCC lattice = $8 \times (\frac{1}{8}) + 6 \times (\frac{1}{2})$

$$= 4 \text{ atoms of one kind (Na)}$$

$$\text{Also } 4 \times (\frac{1}{4}) + 4 \times (\frac{1}{4}) + 4 \times (\frac{1}{4}) + 1$$

$$= 4 \text{ atoms of other kind (Cl)}$$

So four molecules per unit cell in FCC



Diamond Structure

FCC with a basis of two carbon atom one at origin and second at body diagonal

Two interpenetrating FCC lattices

Diamond structure = $FCC_1 + FCC_2$

$FCC_1 \rightarrow$ origin at $(0, 0, 0)$

$FCC_2 \rightarrow$ origin at $(1/4, 1/4, 1/4)$

$(0,1) \rightarrow$ atoms at lower and upper corner

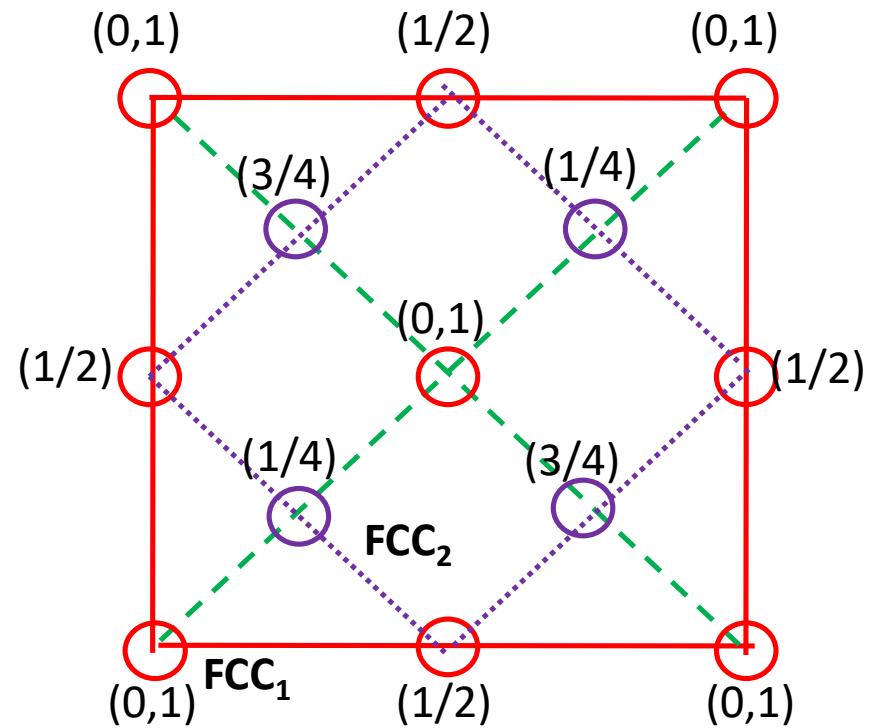
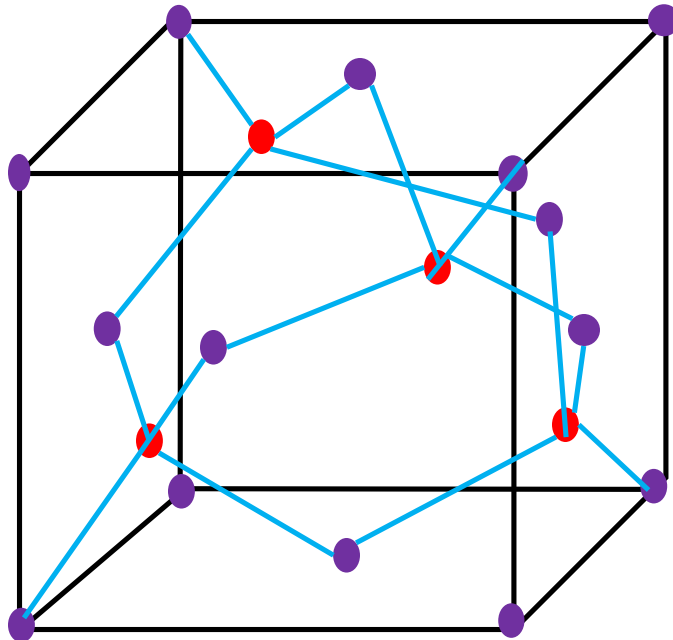
At same position

$(1/2) \rightarrow$ one atom at the lower face center

$(0) \rightarrow$ atom at the center of upper face

$(1/4) \rightarrow$ atom at the body diagonal

$(3/4) \rightarrow$ atom at the other body diagonal



Coordination number=4

Si, Ge, GaAs and Grey Tin have Diamond structure

Zinc Blende (ZnS) structure

The Zinc Blende structure is very similar to Diamond structure
 The only difference here is that one of the FCC lattices is occupied by Zn and the other FCC lattice is occupied by S atom.
 Each atom is attached to four atoms of other type.

Coordination number=4

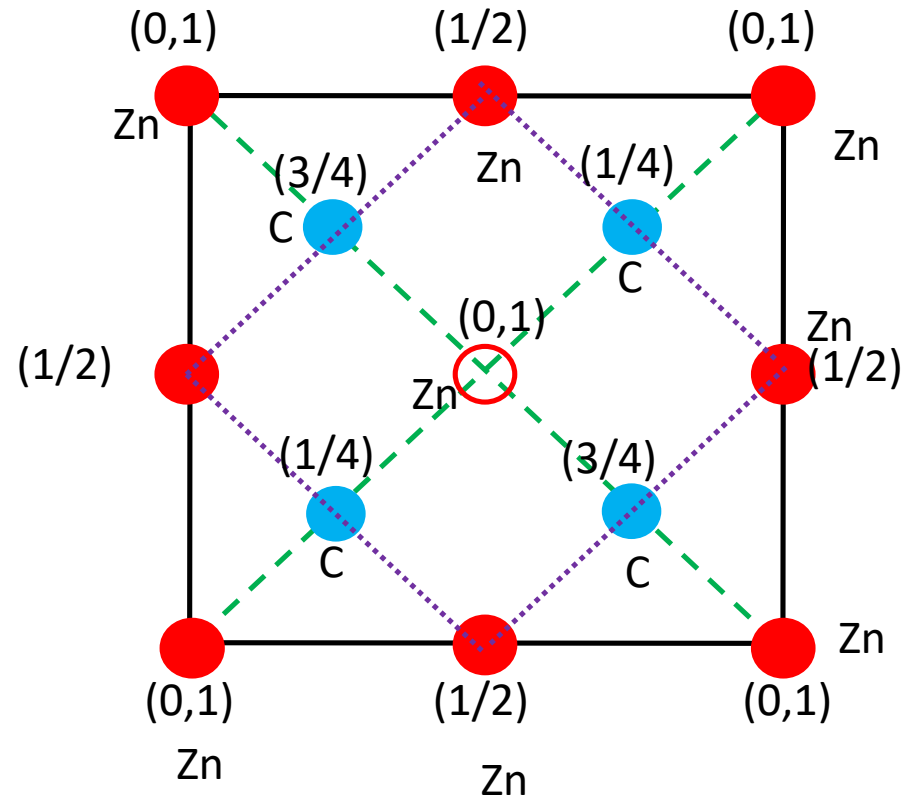
The Zn atoms are shown as red dots

● at $(0, 0, 0)$, $(0, \frac{1}{2}, \frac{1}{2})$, $(\frac{1}{2}, 0, \frac{1}{2})$,
 $(\frac{1}{2}, \frac{1}{2}, 0)$

The S atoms are shown as light blue
 Dots and their coordinates are

● $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$, $(\frac{1}{4}, \frac{3}{4}, \frac{3}{4})$
 $(\frac{3}{4}, \frac{1}{4}, \frac{3}{4})$, $(\frac{3}{4}, \frac{3}{4}, \frac{1}{4})$

Each Zinc atom is surrounded by 4 S atoms
 And each S atom is surrounded by 4 Zn atoms



References:

1. J P Agarwal; Solid state and Nuclear Physics
2. Charles Kittel; Introduction to Solid State Physics