Table 1: Examples of fcc elemental (monatomic) crystal structures

Element	$a(\mathring{A})$	Element	$a(\mathring{A})$
Ar	5.26(4.2K)	Ne	4.43(4.2K)
Ag	4.09	Ni	3.52
Ca	5.58	Pb	4.95
Cu	3.61	Th	5.08

Table 2: Examples of bcc elemental (monatomic) crystal structures

Element	$a(\mathring{A})$	Element	$a(\mathring{A})$
Ba	5.02	Li	3.49(78K)
K	5.23(5K)	Na	4.23(5K)
Cr	2.88	Mo	3.15
Fe	2.87	V	3.02

Questions:

1) How many lattice points are in a unit cell of each of the fcc and bcc Bravais lattices?
2) What is the coordination number of each of fcc and bcc structures?
3) Find the volume of primitive cell in each of the fcc and bcc structures.
4) What is the value of the distance of nearest neighbor for each of the fcc and bcc structures?

[Note: There is two important factors that specifies the most densely crystal structure; these are, (a) the largest PF (b) the highest coordination number].

Packing Fraction (PF) for cubic crystal structures:

Example: Copper crystallizes in a fcc structure.

a) What is the total number of atoms in this structure?

b) Find the PF of this structure.

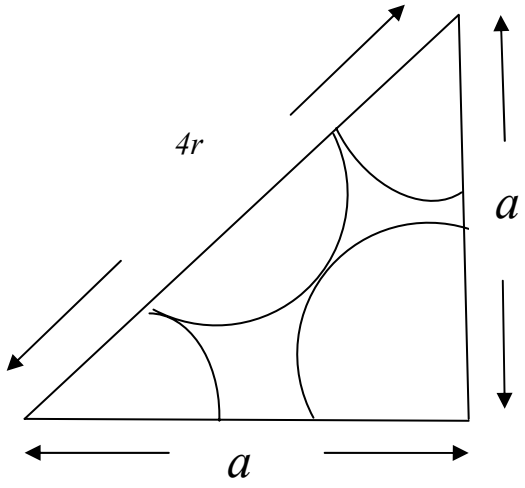

Figure 14: A cross-ection of half-face of the cubic fcc conventional cell.

Solution:

a) The total number of atoms= (1/8 × 8 + 1/2 × 6)= 4 atoms

b) Since $4r = a\sqrt{2}$, thus the distance of nearest neighbor = $\frac{a}{\sqrt{2}}$

, [because $2r$ is the nearest neighbor].

$$PF = \frac{v_{atoms}}{V_{cell}} = \frac{4(\frac{4}{3}\pi r^3)}{a^3}$$

we found that $r = \frac{a}{2\sqrt{2}}$

$$\therefore PF = \frac{16\pi}{3(16\sqrt{2})} = 0.74$$

Table 3: Properties of cubic crystal structures

	sc	bcc	fcc
Lattice points per unit cell	1	2	4
Lattice points per unit volume	$\frac{1}{a^3}$	$\frac{2}{a^3}$	$\frac{4}{a^3}$
Number of nearest neighbors	6	8	12
Nearest neighbor distance	a	$0.86a$	$0.707a$
Number of second neighbors	12	6	6
Second neighbor distance	$1.41a$	a	a
Volume of conventional cell	a^3	a^3	a^3
Volume of primitive cell	a^3	$\frac{a^3}{2}$	$\frac{a^3}{4}$
Packing fraction	0.52	0.68	0.74

Simple hexagonal lattice (sh):

The primitive vectors that form a simple hexagonal Bravais lattice are, $\vec{a}_1 = a\hat{x}$, $\vec{a}_2 = \frac{a}{2}(\hat{x} + \sqrt{3}\hat{y})$ and $\vec{a}_3 = c\hat{z}$, as shown in figure 15. The vectors $\vec{a}_1$ and $\vec{a}_2$ give us the triangular lattice in the x-y plane, while c represents the altitude; this is because a third atom stacks the planes a distance c above another i.e. $c = a = 2r$.

In the conventional *sh* unit cell there are three atoms which contribute as follows:

1. Since there are 12 atoms at the corners that are equally shared between 6 unit cells; thus they contribute a total of two atoms.
2. The atoms in the centers of the top and bottom of the cell are each shared between two unit cells. They contribute a single atom to the cell, [see figure 16].

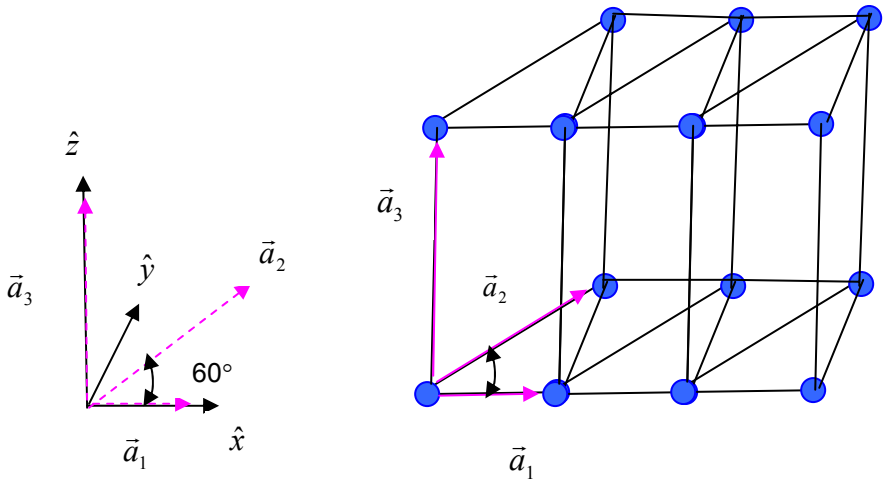

Figure 15: The simple hexagonal (sh) Bravais lattice

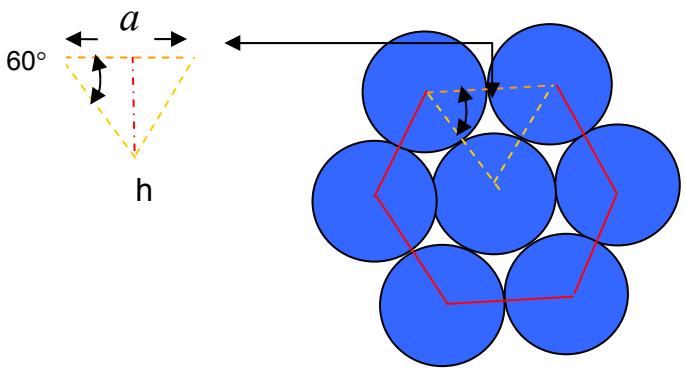

Figure 16: The base of simple hexagonal conventional cell

Example: Find the PF of the simple hexagonal Bravais lattice.

Solution:

The volume of hexagonal unit cell =

The area of the base (hexagon) × Altitude (c)

Area of hexagon = 6 × area of dashed triangle (in figure 16)

$$= 6(\tfrac{1}{2}ha) = \frac{3\sqrt{3}}{2}a^2$$

$$\therefore V_{cell} = \frac{3\sqrt{3}}{2}ca^2$$

we know that $c = a = 2r$

$$\therefore PF = \frac{3(\tfrac{4}{3}\pi r^3)}{\frac{3\sqrt{3}}{2}ca^2} = 0.60$$