Hexagonal close-packed lattice (hcp):

This consists of two interpenetrating simple hexagonal Bravais lattices displaced from one another by $\frac{\vec{a}_1}{3}+\frac{\vec{a}_2}{3}+\frac{\vec{a}_3}{2}$, as shown in figure 17.

[Note: The choice of the primitive vectors in x-y plane of this figure is different from that in figure 23 of "Introduction to Solid State Physics by C. Kittle, where the position vector is defined by $\frac{2\vec{a}_1}{3}+\frac{\vec{a}_2}{3}+\frac{\vec{a}_3}{2}$. However the altitude remains the same in both figures].

The packing fraction of the *hcp* structure is different from that of *sh*.

[Note: Both have the same area of base hexagon which was already determined previously, in the case of *sh*].

However the altitude of *hcp* is different from that of *sh* which can be found as: $c=(\frac{8}{3})^{1/2}a$ [Prove this!!]

The volume of the cell $V_{cell}=4.2426a^3$

The total number of atoms in a unit cell is 6. [i.e. {3/2 (top layer) + 3/2 (bottom layer) + 3 (inside the cell)}.

$\therefore PF=\frac{6(\frac{4}{3}\pi r^3)}{4.2426a^3}=0.74$, where $2r=a$.

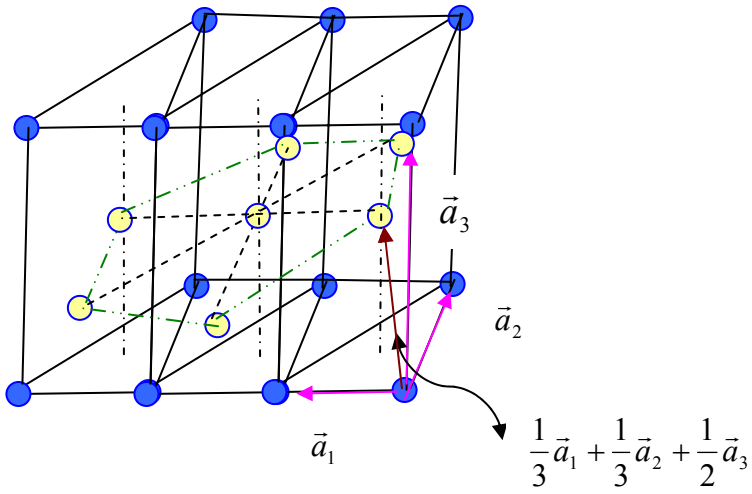

Figure 17: The hexagonal close-packed crystal structure (*hcp*)

Tetrahedral (Diamond) structure:

The conventional unit cell of this structure is *fcc* with a basis of two carbon atoms associated with each lattice site. Each atom has only four nearest neighbors forming a tetrahedral bond. There are eight atoms per a conventional unit cell which are distributed as follows: 6/2 (at faces) + 8/8 (at corners) + 4 (inside) . The whole diamond structure can be visualized as two interpenetrating *fcc* lattices, one displaced from the other by one-fourth the length of cube edge and along a cube diagonal.

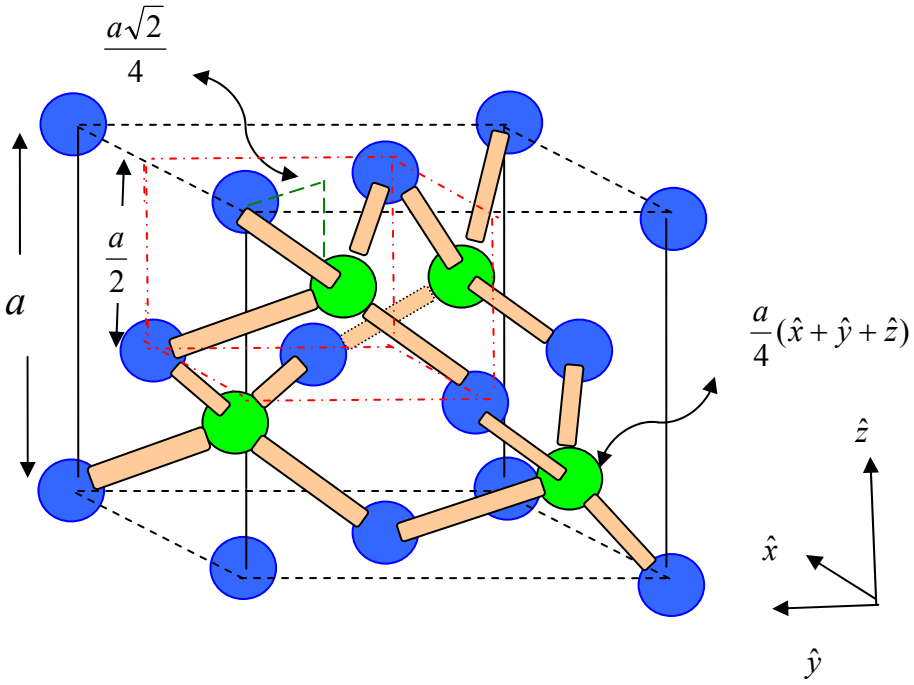

Figure 18: The diamond crystal structure. The green spheres are to indicate the number of atoms inside the conventional cell.

Table 4: Elements with tetrahedral (diamond) structure

Element	**Cube side** $a(\mathring{A})$
C	3.57
Ge	5.66
Si	5.43
Sn	6.49

Example: The dimension of the unit cell the cubic structure of silicon which crystallizes in the diamond structure is 5.43 $\mathring{A}$. The atomic weight of Si is 28.1 g/mole. Find

a) The nearest-neighbor distance between atoms (the bond length).

b) The atomic radius of a silicon atom in this structure.

c) The density of silicon.

Solution:

a) The nearest neighbor distance (named d) can be determined, for example from the upper left tetrahedron. $d = \sqrt{(\frac{a}{4})^2 + (\frac{a\sqrt{2}}{4})^2} \Rightarrow d = \frac{a\sqrt{3}}{4} = 2.35\,\mathring{A}$

b) Since $d = 2r$ $\Rightarrow r = 1.17\,\mathring{A}$.

c) We know that the total atom per unit cell is eight.

The mass per unit cell= Number of atoms per unit cell $\times$ atomic weight / Avogadro number.

Thus the mass per unit cell= $\frac{(8)(28.2)}{6.02\times10^{23}} = 3.73\times10^{-22}$ g.

$\therefore$ The density= mass per unit cell/volume of unit cell

= $3.73\times10^{-22}/ (5.43\times10^{-8})^3 = 2.33$ g. cm^{-3}