Diamond cubic structure -

DC structure - (< 18°C)

Carbon exist in three forms — Diamond, Graphite, Fullernes (70-80 Catom form crystals)

Diamond - $sp^3$ hybridization — inter bond angle 109.5°

Graphite - $sp^2$ hybridization — inter bond angle 120°

Diamond structure consist of two ~~interplanes~~ interpenetrating face centre cubic arrangement of C-atoms. [each carbon atom surrounded by four C-atom sitting at the corners of tetrahedron]

Space lattice of diamond is face centred cubic (FCC) with two atoms per lattice point

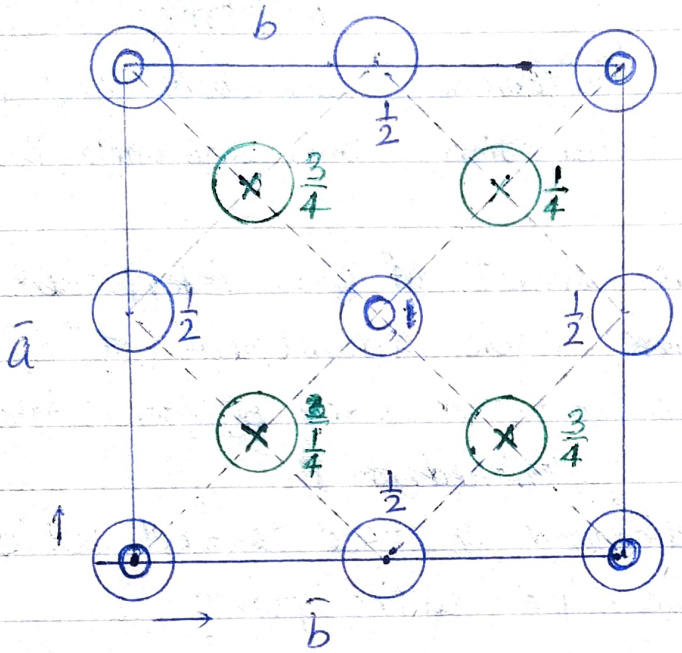
i.e. motif consist of two atoms, one at the corner of unit cell & the other atom at $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ along the body diagonal, which is not a lattice point.

FCC contains 4 lattice point per unit cell

DC consist of 8 lattice point per unit cell

| | | | | | | |
|---|---|---|---|---|---|---|
| 0 | 0 | 0 | $\frac{1}{4}$ | $\frac{1}{4}$ | $\frac{1}{4}$ | add $\frac{1}{4}\ \frac{1}{4}\ \frac{1}{4}$ |
| $\frac{1}{2}$ | $\frac{1}{2}$ | 0 | $\frac{3}{4}$ | $\frac{3}{4}$ | $\frac{1}{4}$ | get another set |
| $\frac{1}{2}$ | 0 | $\frac{1}{2}$ | $\frac{3}{4}$ | $\frac{1}{4}$ | $\frac{3}{4}$ | |
| 0 | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{4}$ | $\frac{3}{4}$ | $\frac{3}{4}$ | |

each atom has four nearest neighbours
next 12 nearest neighbours.
there are 8 atoms per unit cell.
Diamond lattice is relatively empty




Atomic positions in the cubic cell of the diamond structure projected on a cube face

fractions denoted height above the base in units of a cube edge.

The points at 0 & $\frac{1}{2}$ are on the fcc lattice, those at $\frac{1}{4}$ & $\frac{3}{4}$ are on a similar lattice displaced along the body diagonal by one fourth of its length.

with a fcc space lattice, the motif consists of two identical atoms at 000, $\frac{1}{4}\frac{1}{4}\frac{1}{4}$.

packing fraction = $\frac{\text{Volume occupied}}{\text{Volume available}}$

$= \frac{8 \times \frac{4}{3}\pi r^3}{a^3}$

direction of closest approach $\langle 111 \rangle$

Length of body diagonal $= \sqrt{3}\,a$

distance between two nearest neighbours (ie. two motif atom) $= \frac{\sqrt{3}\,a}{4}$

$\therefore 2r = \frac{\sqrt{3}}{4} a \qquad a = \frac{8r}{\sqrt{3}}$

$p.f = \frac{8}{8} \times \frac{4}{3}\pi r^3 \times \frac{8\sqrt{3}}{8 \times 8 \times 8 \times r^3} = \frac{\pi\sqrt{3}}{16} = 0.34$

ie. only 34% space occupied

so open structure.

Carbon, Ge, Si, & gray tin crystallize in the diamond structure.

Diamond structure - highly directional

Co-valent bonding

| Element | Lattice type | Motif | Nb. of Atoms per unit cell | Direction of closest approach | p.f. | no. of N. neighbours. | Closed pack plane |
|---|---|---|---|---|---|---|---|
| Cu, Ag, Au, Al | FCC | one atom (000) | 4 (000) $(\frac{1}{2}\frac{1}{2}0)$ $(0\frac{1}{2}\frac{1}{2})$ $(\frac{1}{2}0\frac{1}{2})$ | $\langle 110 \rangle$ | .74 | 12 | {111} |
| Zn, Cd, Ti | HCP | Two atoms (000) $(\frac{1}{3}\frac{2}{3}\frac{1}{2})$ | Two | $\langle 11\bar{2}0 \rangle$ | .74 | 12 | (0001). |
| Na, K, Li Nb, Ta | BCC | one atom (000) | Two (000) $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ | $\langle 111 \rangle$ | .68 | 8 | {110} |
| Po | SC | one atom (000) | One | $\langle 100 \rangle$ | .52 | 6 | {100} |
| C (diamond) gray Tin Si, Ge | DC | two atoms 000 $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ | 8 000 $0\frac{1}{2}\frac{1}{2}$ $\frac{1}{2}0\frac{1}{2}$ $\frac{1}{2}\frac{1}{2}0$ $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ $\frac{1}{4}\frac{3}{4}\frac{3}{4}$ $\frac{3}{4}\frac{1}{4}\frac{3}{4}$ $\frac{3}{4}\frac{3}{4}\frac{1}{4}$ | $\langle 111 \rangle$ | .34 | 4 | {110} |