Diamond Crystal Structure

Diamond is a metastable allotrope of carbon where the each carbon atom is bonded covalently with other surrounding four carbon atoms and are arranged in a variation of the face centered cubic crystal structure called a diamond lattice

Diamond Unit Cell

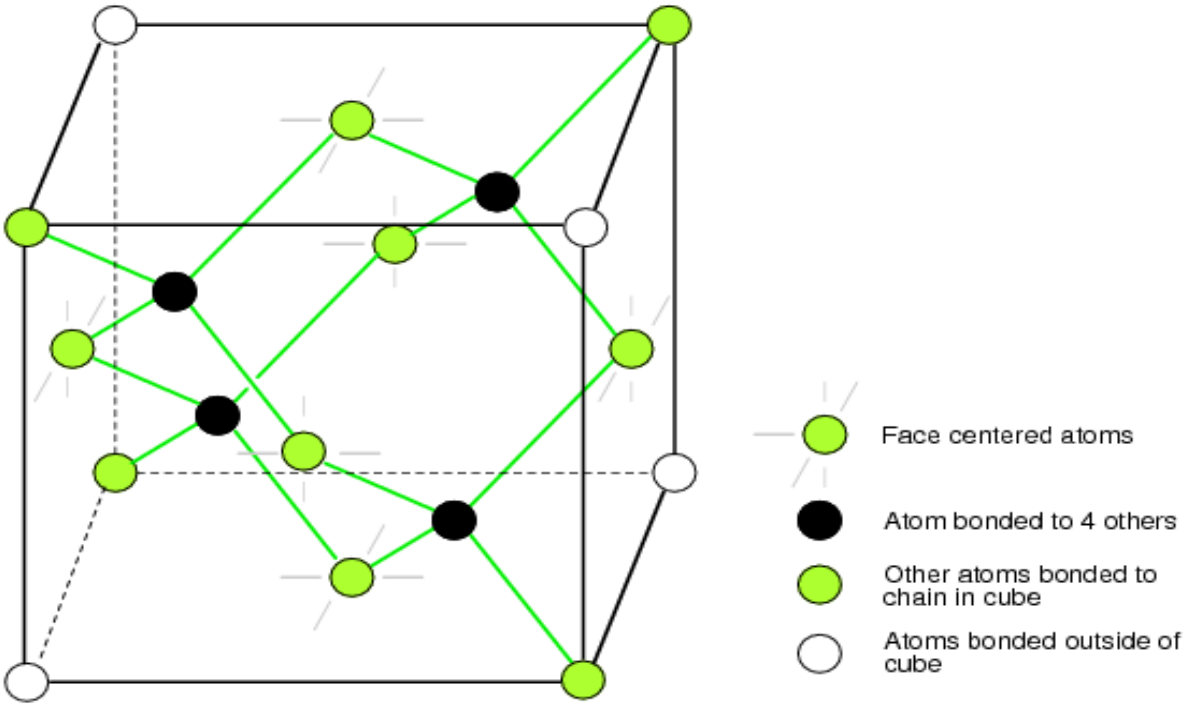
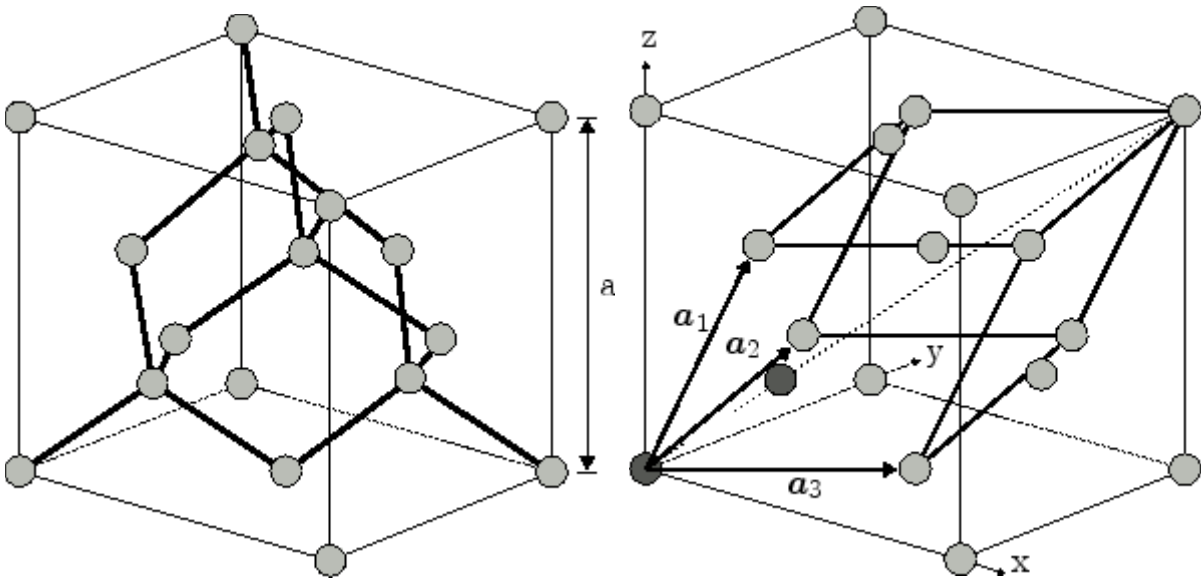


Figure shows four atoms (dark) bonded to four others within the volume of the cell. Six atoms fall on the middle of each of the six cube faces, showing two bonds. Out of eight cube corners, four atoms bond to an atom within the cube. The other four bond to adjacent cubes of the crystal

Lattice Vector and Basis Atoms

So the structure consists of two basis atoms and may be thought of as two inter-penetrating face centered cubic lattices, with a basis of two identical carbon atoms associated with each lattice point one displaced from the other by a translation of ao(1/4,1/4,1/4) along a body diagonal so we can say the diamond cubic structure is a combination of two interpenetrating FCC sub lattices displaced along the body diagonal of the cubic cell by 1/4th length of that diagonal. Thus the origins of two FCC sub lattices lie at (0, 0, 0) and (1/4, 1/4,1/4)



(a) (b)

(**a**) Crystallographic unit cell (unit cube) of the diamond structure (**b**) The primitive basis vectors of the face centered cubic lattice and the two atoms forming the basis are highlighted.

The primitive basis vectors and the two atoms at (0,0,0) and ao(1/4,1/4,1/4) are highlighted in Figure(b)and the basis vectors of the direct Bravais lattice are

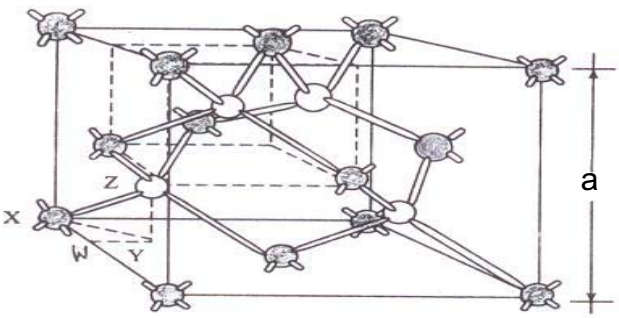
$$\boldsymbol{a}_1 = \frac{a_0}{2}\begin{pmatrix}0\\1\\1\end{pmatrix}\ , \quad \boldsymbol{a}_2 = \frac{a_0}{2}\begin{pmatrix}1\\0\\1\end{pmatrix}\ , \quad \text{and} \quad \boldsymbol{a}_3 = \frac{a_0}{2}\begin{pmatrix}1\\1\\0\end{pmatrix}\ ,$$

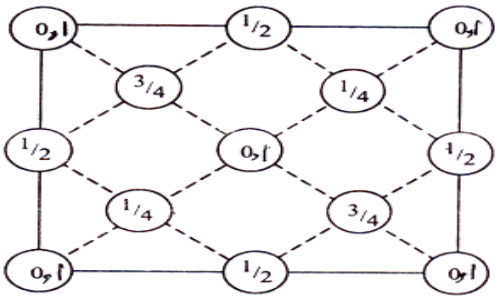
Where ao denotes the lattice constant of the relaxed lattice. The lattice is invariant under translations involving lattice vectors of the form

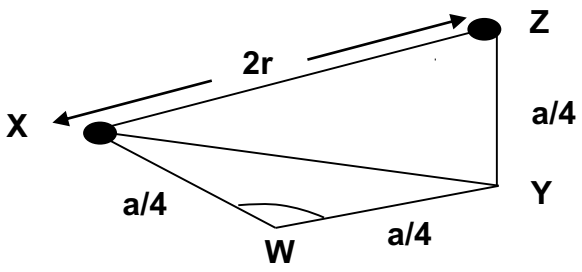
$$\boldsymbol{R}_{ijk} = i\boldsymbol{a}_1 + j\boldsymbol{a}_2 + k\boldsymbol{a}_3\ ,$$

where i , j and k are integers.

Number of atoms contributed by the corner atoms to an unit cell is 1/8×8 =1 and number of atoms contributed by the face centred atoms to the unit cell is 1/2 × 6 = 3 and atoms inside the structure =4 ,so total number of atoms present in a diamond cubic unit cell is 1 + 3 + 4 = 8,Since each carbon atom is surrounded by four more carbon atoms,the co-ordination number is 4







From triangle WXY

XY^2=(a/4)^2+(a/4)^2

=(a^2)/8

From triangle XYZ

XZ^2=(a^2)/8 + (a/4)^2

=(3a^2)/16

But XZ=2r

So (2r)^2 = (3a^2)/16

Atomic radius r =(a(3)^1/2)/8

Atomic packing factor is = v/V

=[(8*4*PI*r^3)/3]/[(a)^3]

By putting value of r we get-----

APF=0.34 =34%

Thus it is a loosely packed structure