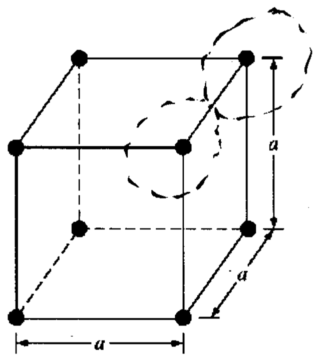
1.2 Assume that each atom is a hard sphere with the surface of each atom in contact with the surface of its nearest neighbor. Determine the percentage of total unit cell volume that is occupied in (*a*) a simple cubic lattice, (*b*) a face-centered cubic lattice, (*c*) a body-centered cubic lattice, and (*d*) a diamond lattice.

- Also, determine the number of atoms per unit cell in each case.

a)



Here, the closest neighbors are at the corners of the cube,

Therefore, $a = r + r = 2r$ (r is radius of each atom)

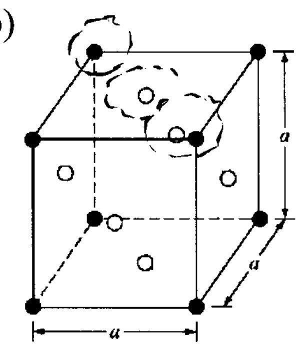
$\hookrightarrow r = a/2$

$$\#\text{ atoms in unit cell} = 8 \text{ corners}\left(\frac{1/8 \text{ atom}}{\text{corner}}\right) = \underline{1 \text{ atom}}$$

cube volume $= a^3$ atom volume $= (1 \text{ atom})\, 4/3\, \pi r^3$

$$\%\text{ unit cell occupied} = \frac{4/3\,\pi (a/2)^3}{a^3}(100\%) = \underline{\underline{52.36\%}}$$

b)



Here, the closest neighbors are along the diagonal of the faces of the cube. Therefore,

$$\text{diagonal} = \sqrt{a^2 + a^2} = r + 2r + r$$

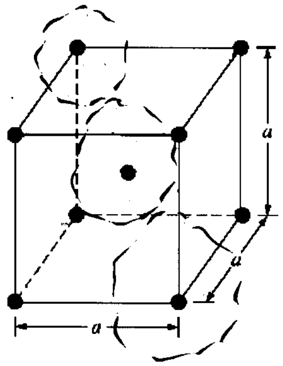
$$\sqrt{2}\, a = 4r \rightarrow r = \frac{\sqrt{2}}{4} a$$

$$\#\text{ atoms in unit cell} = 8 \text{ corners}\left(\frac{1/8 \text{ atom}}{\text{corner}}\right) + 6 \text{ faces}\left(\frac{1/2 \text{ atom}}{\text{face}}\right) = \underline{\underline{4 \text{ atoms}}}$$

cube volume $= a^3$ 4 atoms volume $= (4)\, 4/3\, \pi r^3$

$$\%\text{ unit cell occupied} = \frac{(4)\, 4/3\, \pi \left(\frac{\sqrt{2}}{4} a\right)^3}{a^3}(100\%) = \underline{\underline{74.05\%}}$$

c)



Here, the closest neighbors are along the diagonal of the cube. Therefore,

$$\text{diagonal} = \sqrt{a^2+a^2+a^2} = r + 2r + r$$

$$\sqrt{3}\,a = 4r \rightarrow r = \frac{\sqrt{3}}{4}a$$

$$\#\text{ of atoms in unit cell} = 8\text{ corners}\left(\frac{1/8\text{ atom}}{\text{corner}}\right) + 1\text{ atom} = \underline{\underline{2\text{ atoms}}}$$

cube volume $= a^3$ 2 atoms volume $= (2)\,\frac{4}{3}\pi r^3$

$$\%\text{ unit cell occupied} = \frac{(2)\,\frac{4}{3}\pi\left(\frac{\sqrt{3}}{4}a\right)^3}{a^3}(100\%) = \underline{\underline{68.02\%}}$$

d)

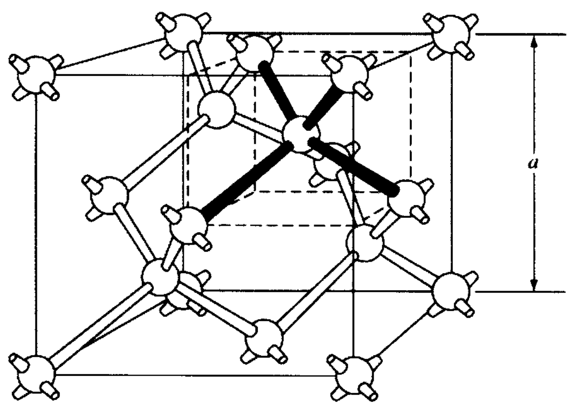


Figure 1.11 | The diamond structure.

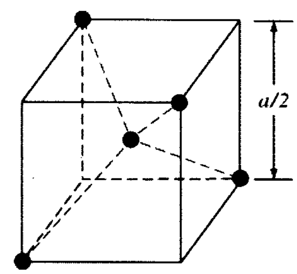


Figure 1.12 | The tetrahedral structure of closest neighbors in the diamond lattice.

From Fig 1.12, the nearest neighbor is along <u>tetrahedron</u> diagonal. Therefore,

$$\text{diagonal} = \sqrt{(a/2)^2+(a/2)^2+(a/2)^2} = \sqrt{\frac{3a^2}{4}} = \sqrt{3/4}\;a = r+2r+r$$

$$\hookrightarrow r = \tfrac{1}{4}\sqrt{3/4}\;a$$

$$\#\text{atoms per unit cell} = 8\text{ corners}(1/8) + 6\text{ faces}(1/2) + 4\text{ interior} = \underline{\underline{8\text{ atoms}}}$$

$$\%\text{ unit cell occupied} = \frac{(8)\,\frac{4}{3}\pi\left(\frac{1}{4}\sqrt{3/4}\,a\right)^3}{a^3}(100\%) = \underline{\underline{34.01\%}}$$