7)

$$\underline{a}_1 = \frac{a}{2}(-\hat{\underline{x}} + \hat{\underline{y}} + \hat{\underline{z}})$$

$$\underline{a}_2 = \frac{a}{2}(\hat{\underline{x}} - \hat{\underline{y}} + \hat{\underline{z}})$$

$$\underline{a}_3 = \frac{a}{2}(\hat{\underline{x}} + \hat{\underline{y}} - \hat{\underline{z}})$$

$$\underline{a}_1 \cdot \underline{a}_1 = \underline{a}_2 \cdot \underline{a}_2 = \underline{a}_3 \cdot \underline{a}_3 = \frac{3a^2}{4}$$

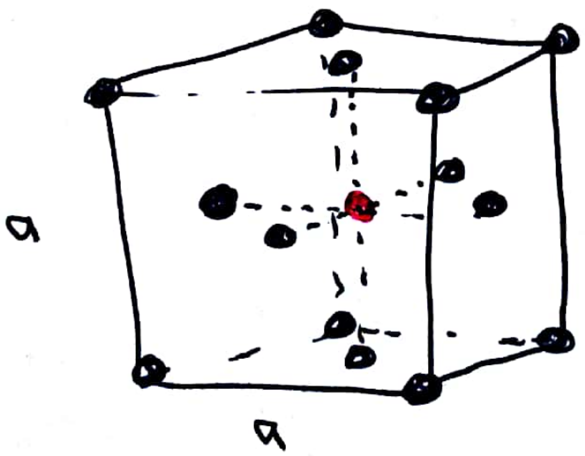
$$\underline{a}_1 \cdot \underline{a}_2 = \frac{a^2}{4}(-1-1+1) = -\frac{a^2}{4} = \underline{a}_2 \cdot \underline{a}_3 = \underline{a}_3 \cdot \underline{a}_1$$

$\therefore$ all three angles are the same:

$$\cos\theta = + \frac{\underline{a}_i \cdot \underline{a}_j}{(3a^2/4)} = -1/3$$

$$\Rightarrow \quad \theta = \cos^{-1}(-1/3) = 1.91 \text{ radians}$$
$$= 72.5^\circ.$$

8)



The red point has 4 nearest neighbours a distance $a/2$ away and 8 next-to-nearest neighbours at the vertices, a distance $\frac{\sqrt{3}a}{2}$ away.

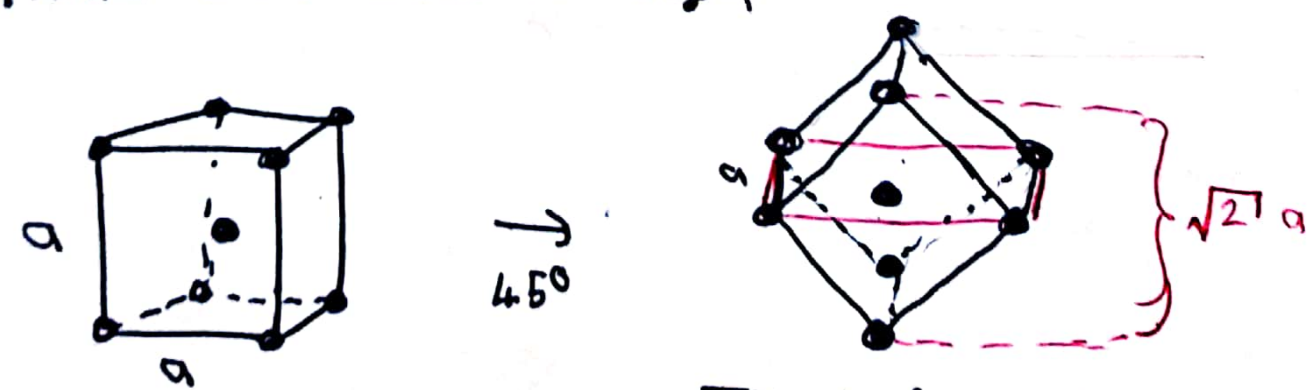
a point on a vertex has 3 nearest neighbours a distance $\frac{a}{\sqrt{2}}$ away, 4 on each of the 3 planes passing through it, and 8 next-to-nearest neighbours (red points at the centres of the 8 cubes that share it as a vertex).

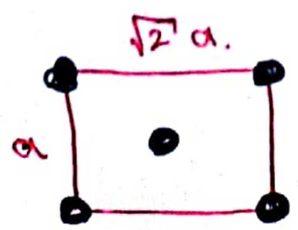
Only the next-to-nearest neighbours of the red and black points are the same. Their nearest neighbours are different — they are not equivalent points and this is not a lattice.

(9) (An orthorhombic lattice with $b=c$ is a tetragonal lattice).

~~a tetragonal lattice with c~~

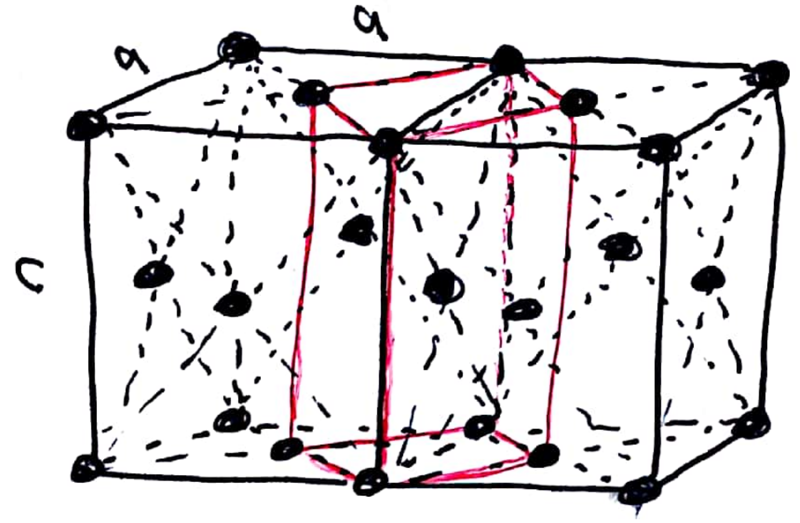
Rotate BCC about an edge:

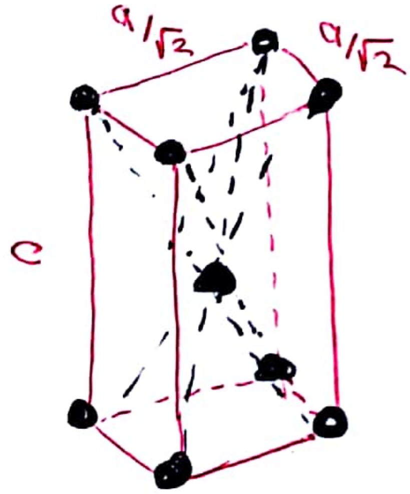




This is face centred orthorhombic with $a=b$ and $c=\sqrt{2}\,a$. (the red rectangle is a face).

10)



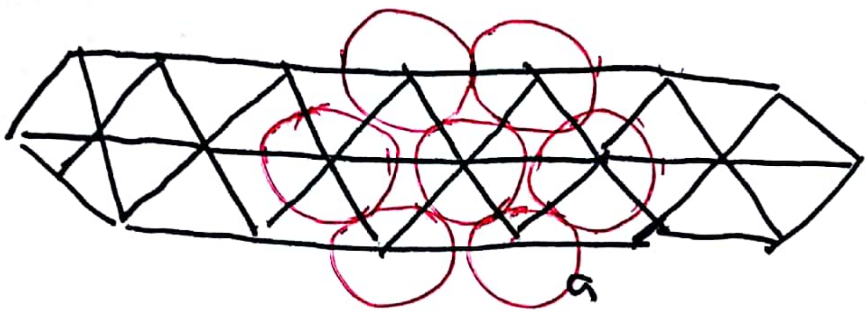


upper figure : two conventional cells of a face-centred rectangular lattice

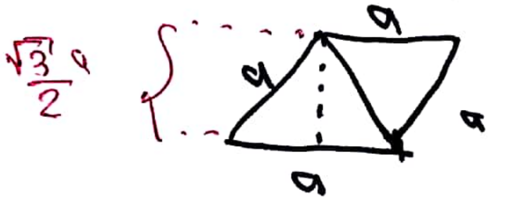
lower figure : one primitive cell of a body centred rectangular lattice.

For the special case $c = a$, a face-centred cubic lattice is equivalent to a body centred rectangular lattice with the top face being a square of side $a/\sqrt{2}$: this is not BCC!

11) i) 2-d hexagonal lattice



Place a circle of radius $a/2$ at the vertices of each equilateral triangle with side a. Primitive cells are rhombi of side a (2 equilateral triangles)



Primitive cells have area $2 \times \frac{a}{2} \times \frac{\sqrt{3}}{2}a = \sqrt{3}\,a^2/2$

Each primitive cell contains one complete circle of area $\pi\left(\frac{a}{2}\right)^2 = \pi a^2/4$

$\therefore$ Packing ~~fr~~ fraction $= \dfrac{\pi a^2/4}{\sqrt{3}\,a^2/2} = \pi/2\sqrt{3}$.

ii) As described in the lectures, diamond is a face centred cubic lattice with a basis consisting of two carbon atoms a distance $\frac{\sqrt{3}a}{4}$ apart, put one atom at the origin and the other at $\frac{a}{4}(\hat{x}+\hat{y}+\hat{z})$: one quarter of the way to the opposite corner of a conventional cell of side a.

If the atoms are a distance $\frac{\sqrt{3}a}{4}$ apart and we model them as hard spheres that touch each other then their radius is $\frac{\sqrt{3}a}{8}$ and each has volume $\frac{4}{3}\pi\left(\frac{\sqrt{3}a}{8}\right)^3 = \frac{\sqrt{3}}{128}\pi a^3$. The basis is two atoms with a total volume $\frac{\sqrt{3}}{64}\pi a^3$.

The conventional side of a FCC lattice with side a contains 4 primitive cells, so a primitive cell has volume $a^3/4$.

$$\text{Packing fraction} = \frac{\sqrt{3}}{64}\pi a^3 \Big/ a^3/4 = \frac{\sqrt{3}\pi a^3}{16}.$$

(12) Face-centred cubic has nearest neighbour separation $a/\sqrt{2}$ in a conventional cell of side a

$\Rightarrow$ touching spheres at each lattice site have radius $\frac{a}{2\sqrt{2}}$ and volume $\frac{4}{3}\pi\left(\frac{a}{2\sqrt{2}}\right)^3 = \frac{\pi a^3}{3\times 4\sqrt{2}}$

Conventional cell has side a, volume a^3, and contains four primitive cells $\Rightarrow$ volume of a primitive cell is $a^3/4$

Packing fraction $= \frac{\pi a^3}{4\times 3\sqrt{2}} \Big/ a^3/4 = \pi \cdot \frac{1}{3\sqrt{2}}$

Model lead atom as a sphere with radius 1.75×10^{-10} m and mass 207.2 a.m.u $= 3.44\times 10^{-25}$ kg.

$\Rightarrow$ the density of a lead atom is

$$\rho_a = \frac{3.44\times 10^{-25}}{\frac{4\pi}{3}(1.75\times 10^{-10})^3}\ \text{kg m}^{-3} = 0.1532\times 10^{5}\ \text{kg m}^{-3}$$

$$= 15.32\ \text{g/cc}$$

Packing fraction $= \frac{\sqrt{2}\pi}{6} = 0.74$

$\Rightarrow$ density of lead $= \frac{\sqrt{2}\pi}{6} \times 15.32$ g/cc

$= 11.3$ g/cc