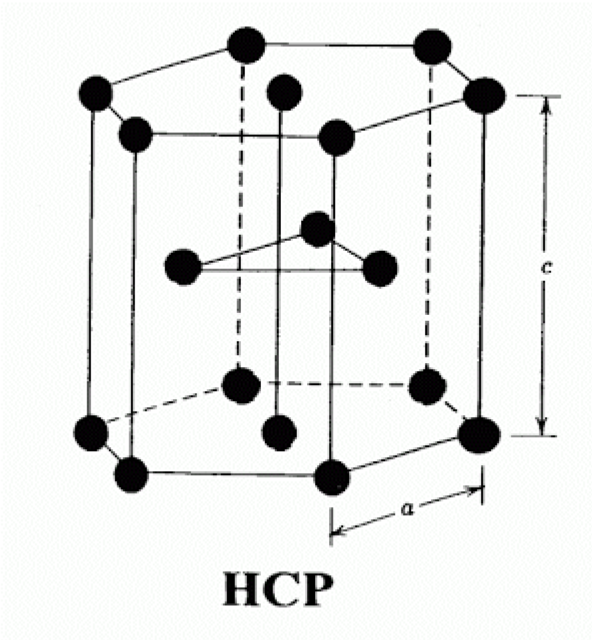
Hexagonal Closed Packing Structure **S.J.Eichhorn 15/02/18**

The Atomic Packing Factor is defined by the equation

$$Atomic\ Packing\ Factor = \frac{Volume\ of\ atoms\ in\ cell\ (v)}{Volume\ of\ total\ cell\ (V)}$$

[Note: definitions of v and V are given in brackets in the equation]



A Hexagonal closed packed structure has a unit cell looks like the image on the left. The basic unit cell however encloses the 3 atoms at the centre (in black) and shares the upper and lower planes of atoms (white) with surrounding unit cells.

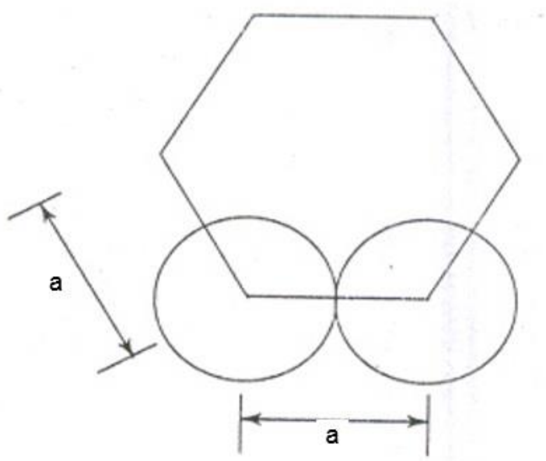
So, in the unit cell we have 3 middle atoms. The 6 outer atoms in the planes (white) are shared with adjacent cells, leaving 1/6th of each in the unit cell. The central atoms in the top and bottom planes (white) are shared by cells top and bottom of the cell shown left.

So, we have

Number of atoms = 3 +(1/2)*2 + (1/6)*2 = 6 atoms in the unit cell.

$$Volume\ of\ atoms\ in\ unit\ cell = 6\ \times \frac{4}{3}\pi r^3$$

Given that a = 2r, which is best viewed from the projection below (Note: in the cell atoms are touching each other - so the closed packed structure is a set of touching spheres.



If we consider the two corner atoms. The APF can be written as

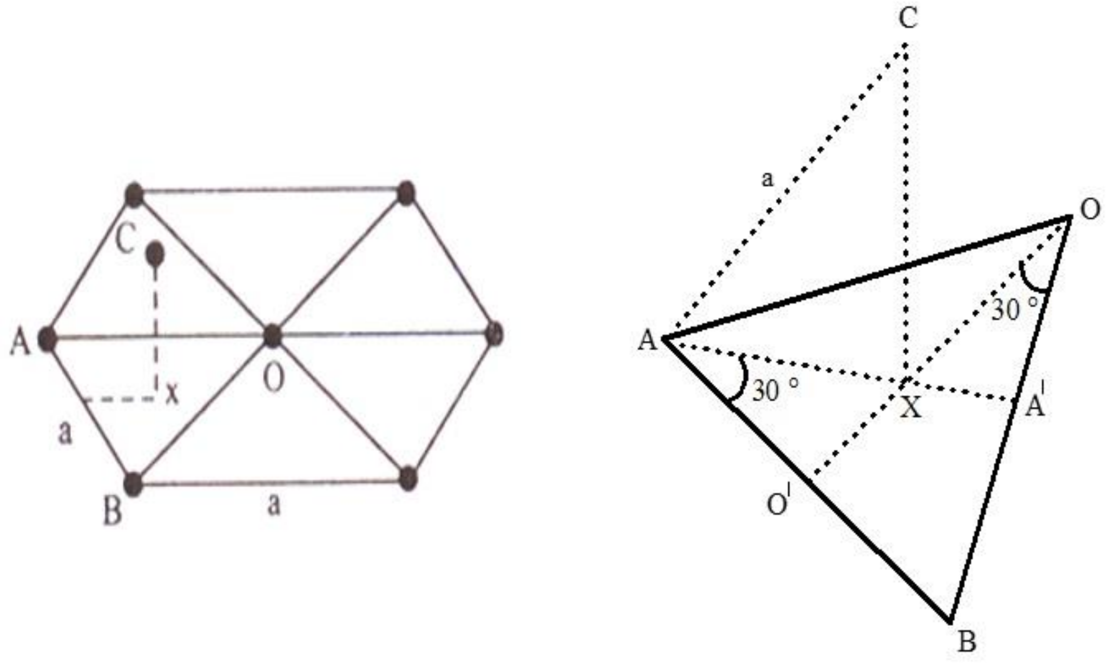
$$APF = \frac{v}{V}$$

Where $v = 6\ \times \frac{4}{3}\pi r^3$

If we substitute in a=2r into this (or r = a/2) then we obtain

$$v = 6 \times \frac{4}{3} \times \pi \frac{a^3}{8} = \pi a^3$$

So, looking at the projections given the following geometries



Where the base of the closed packed structure is in effect a set of six equilateral triangles (left hand image).

The area of the base of the hexagonal structure is given by

$$Area\ of\ hexagonal\ base = 6\ \times area\ of\ the\ triangle\ ABO$$

[Note: we just use the area of the triangle ABO here but all the triangles in the base are equal so it does not matter which one is chosen.

The right-hand image above shows one triangle (again ABO) with the intersections splitting into two right angled triangles (30°+60°+90° = 180°) – these intersections are given by AA' and O'O. Above a point X, where these lines intersect, at a height of c/2 is another atom.

In the triangle OBO' the angle O'ÔB = 30°

$$\cos 30° = \frac{OO'}{BO} = \frac{OO'}{a}$$

Therefore,

$$OO' = \text{a}\cos 30° = a\frac{\sqrt{3}}{2}$$

$$Area\ of\ base = 6 \times \frac{1}{2} \times a \times \frac{\sqrt{3}}{2} a = \frac{3\sqrt{3}a^2}{2}$$

$$Volume\ of\ hexagonal\ structure = Area\ of\ base\ \times height$$

$$= \frac{3\sqrt{3}a^2}{2} \times c$$

So,

$$APF = \frac{v}{V} = \frac{\pi a^3}{\frac{3\sqrt{3}a^2}{2} \times c} = \frac{2\pi}{3\sqrt{3}} \frac{a}{c}$$

The angle AÂ’B = 30°

So,

$$\cos 30° = \frac{AA'}{AB}$$

Therefore,

$$AA' = AB \cos 30° = a\frac{\sqrt{3}}{2}$$

But,

$$AX = \frac{2}{3}AA' = \frac{2}{3}a\frac{\sqrt{3}}{2}$$

[Note: why is $AX = \frac{2}{3}AA'$? Well, if you take the following equations

$$\sin 30° = \frac{O'X}{AX}$$

$$\sin 30° = \frac{A'B}{AB}$$

Therefore

$$\frac{O'X}{AX} = \frac{A'B}{AB} = \frac{\frac{a}{2}}{a} = \frac{1}{2}$$

and

$$AX^2 = (AO')^2 + (O'X)^2$$

$$AX^2 = (\frac{a}{2})^2 + (O'X)^2$$

Since we know that

$$O'X = \frac{1}{2}AX$$

then,

$$AX^2 = \frac{a^2}{4} + \frac{1}{4}(AX^2)$$

$$\frac{3}{4}AX^2 = \frac{a^2}{4}$$

Therefore,

$$AX = \frac{a}{\sqrt{3}}$$

Using Pythagoras,

$$(AB)^2 = (A'B)^2 + (AA')^2$$

Now we know that,

$$AB = a \; and \; A'B = \frac{a}{2}$$

So,

$$(AA')^2 = a^2 - \frac{a^2}{4} = \frac{3a^2}{4}$$

$$AA' = \frac{\sqrt{3}a}{2}$$

Therefore,

$$\frac{AX}{AA'} = \frac{\frac{a}{\sqrt{3}}}{\frac{\sqrt{3}a}{2}} = \frac{2}{3}$$

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In the triangle AXC,

$$AC^2 = AX^2 + CX^2$$

So,

$$a^2 = \left(\frac{a}{\sqrt{3}}\right)^2 + \left(\frac{c}{2}\right)$$

[Note: CX is half way up the full structure so equal to c/2]

Rearranging and solving for c gives,

$$c = a\sqrt{\frac{8}{3}}$$

Therefore, APF is found by,

$$APF = \frac{2\pi}{3\sqrt{3}}\frac{a}{c} = \frac{2\pi}{3\sqrt{3}}\frac{a\sqrt{3}}{a\sqrt{8}} = \frac{2\pi}{3\sqrt{8}} = \frac{6.28}{8.49} = 0.74$$