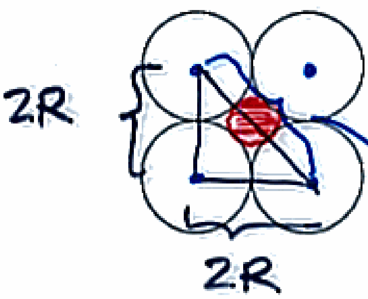
How big are tetrahedral, octahedral and cubic holes?

Let's look at octahedral holes first.



Let r_o be the radius of a sphere that just fits into the octahedral hole.

$R + 2r_o + R$

$$(2R)^2 + (2R)^2 = (2R + 2r_o)^2$$

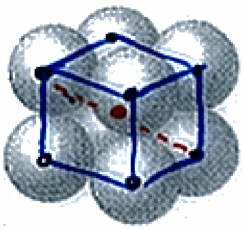
$$8R^2 = 4(R + r_o)^2$$

$$\therefore \sqrt{2}R = R + r_o$$

$$r_o = (\sqrt{2} - 1)R = 0.414R$$

Note: If the radius of the sphere in the octahedral hole is greater than 0.414 R, then the spheres forming the octahedron will be pushed apart.

And now for cubic holes ...



Let r_c be the radius of a sphere that just fits into the cubic hole. Note that this small sphere has its centre at the midpoint of the body-diagonal ∴ need to find length of BD.

Recall: $BD^2 = 3\,edge^2$ (for any cube)

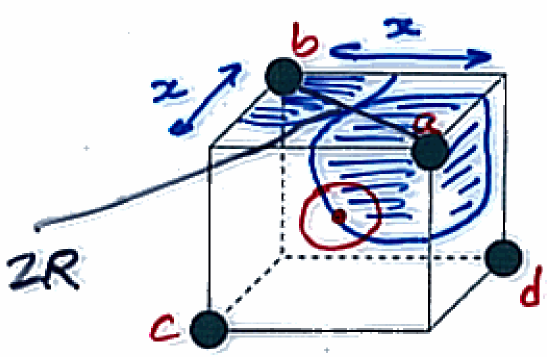
$$\therefore \quad BD^2 = 3(2R)^2$$
$$BD = 2\sqrt{3}\,R$$

But $BD = R + 2r_c + R = 2R + 2r_c$

$$\therefore \quad 2R + 2r_c = 2\sqrt{3}\,R$$
$$r_c = (\sqrt{3} - 1)R$$
$$\simeq 0.732\,R$$

If the sphere at the centre of cube, ~~the~~ has $r > 0.732R$, the spheres forming the cubic hole will be pushed apart.

And finally, tetrahedral holes ... (see p. 18)



Note: The large spheres (of radius R) are in direct contact with each other along the face-diagonals.

Let r_t be the radius of a small sphere that just fits into the tetrahedral hole located at the centre of this cube.

Again, need to find length of BD.

$$x^2 + x^2 = (2R)^2 \Rightarrow x = \sqrt{2}R$$

Recall: $3\,\text{edge}^2 = BD^2$ (any cube)

$$3(\sqrt{2}R)^2 = BD^2$$

$$\therefore BD = \sqrt{6}R$$

But $\frac{1}{2}BD = r_t + R$ (from diagrams above)

$$\frac{1}{2}\sqrt{6}R = r_t + R$$

$$r_t = \left(\frac{\sqrt{6}}{2} - 1\right)R \simeq 0.225R$$

If radius of sphere in tetrahedral site is greater than 0.225 R, then the spheres forming the tetrahedron are pushed apart.