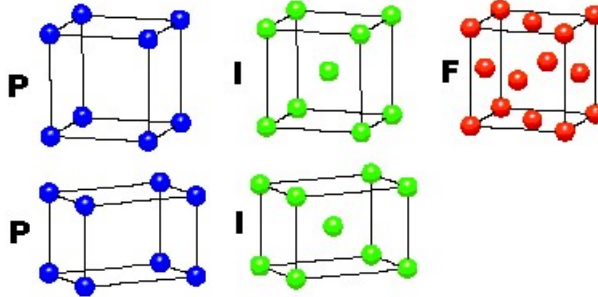


1. A tetragonal lattice is produced by reducing the symmetry of a cubic lattice as shown below ( $c \neq a$ ). That is, by taking a cubic lattice and stretching it along one direction, namely the  $c$ -axis. Here I denotes body-centered, and F denotes face-centered lattices.

**CUBIC**

$$a = b = c$$

$$\alpha = \beta = \gamma = 90^\circ$$



**TETRAGONAL**

$$a = b \neq c$$

$$\alpha = \beta = \gamma = 90^\circ$$

- (a) Obviously, the body-centered tetragonal (BCT) may be produced by stretching the BCC lattice along the  $c$ -axis. Perhaps not so obviously, it may also be produced by stretching the FCC lattice along the same direction. Show (with illustrations if you like) that the BCT lattice may be viewed as a stretched FCC. Show that for  $c/a = \sqrt{2}$  it is identical to FCC. (Hint: look at neighboring planes perpendicular to the  $c$ -axis.)

The figure below shows the BCT lattice planes along the  $c$ -axis. The white atoms are in one plane, whereas the black atoms are in a parallel plane, a distance  $c/2$  away. The next plane of white atoms would be a further  $c/2$  away, and so forth. The view on the RHS is that of the BCT as a stretched BCC.

Note that the LHS view is identical in terms of atomic placement and is therefore the same BCT lattice. However it is rotated by  $45^\circ$  and considers four neighboring unit cells.

In this view the plane of white atoms comprises a face-centered square lattice with spacing  $a' = a\sqrt{2}$ .

The black atoms are now at the face centers of rectangles in the perpendicular planes (parallel to the  $c$ -axis).

This is therefore a stretched FCC. A 3-D picture is also shown below.

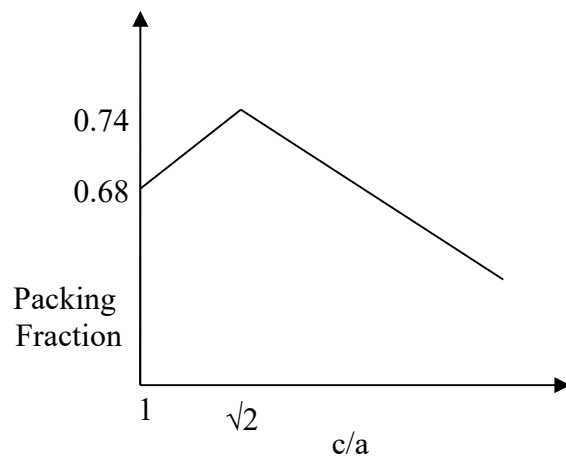
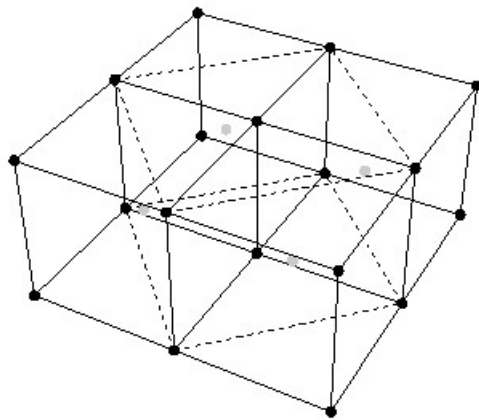
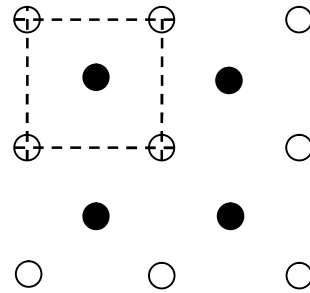
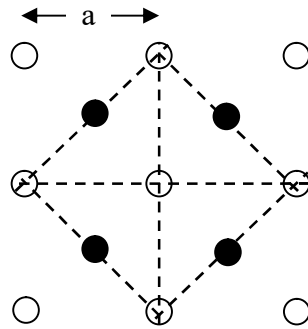
Here the distance from a black atom to the plane of white atoms is  $c/2$ .

This becomes FCC with spacing  $a' = a\sqrt{2}$  when  $c/2 = a'/2 \Rightarrow c = a\sqrt{2}$ .

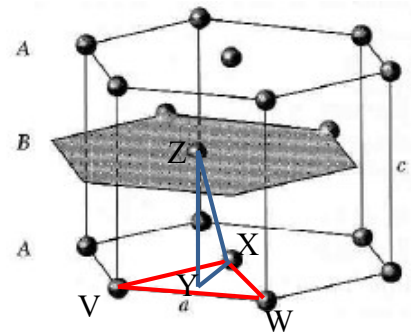
- (b) Sketch schematically the packing fraction for the BCT lattice as a function of  $c/a$  (for  $c \geq a$ ), assuming close-packing.

For  $c = a$ , the BCT becomes BCC with a 68% packing fraction. For  $c = a\sqrt{2}$ , it becomes FCC with a packing fraction of 74% which is the maximum possible. As

$c/a$  increases beyond that, the packing fraction decreases, because the volume of the unit cell keeps increasing without any change in the atomic volumes. A schematic plot is shown below.



2. Consider now the hexagonal close-packed (hcp) crystal structure illustrated below (including layer B now). It consists of two interpenetrating simple hexagonal lattices labeled A and B. For ideal 'close-packing', imagine hard spheres at every lattice point that just touch the neighboring spheres. What is the  $c/a$  ratio in this case? What happens if  $c/a$  is much greater than this value? Can you provide an example of this situation in nature?



Suppose the centre of the hexagon on plane A is X, and the centre of the hexagon in plane B is Z. Consider the perpendicular dropped from Z onto the plane A. It meets the plane A in Y, viz. the centroid of the equilateral triangle VWX.

Each side of the equilateral triangle is  $a$ . Therefore  $XY = \frac{2}{3} \frac{\sqrt{3}}{2} a = \frac{a}{\sqrt{3}}$ .

The height of the perpendicular  $YZ = c/2$ .

Obviously,  $XZ = 2r$  for close packing, where  $r$  is the radius of each atom.

Considering the right angled triangle XYZ, we have:

$$(2r)^2 = \left(\frac{a}{\sqrt{3}}\right)^2 + (c/2)^2 \dots [1]$$

Close packing of the atoms at points X and V in the A-plane implies that  $2r = a$ . Using this we may write Eq. 1 as:

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

$$\text{Therefore, } \frac{2a^2}{3} = \frac{c^2}{4} \Rightarrow \frac{c}{a} = \sqrt{\frac{8}{3}}$$

If this ratio is much greater, then the solid is no longer close packed in the vertical direction, but rather comprises loosely stacked hexagonal sheets. An example is graphite, viz. pencil lead.