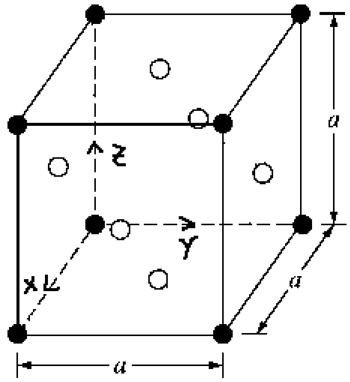
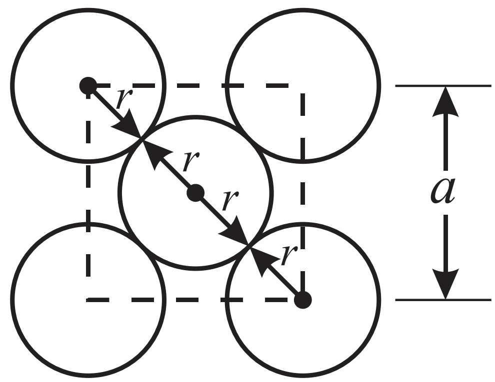
1.21 Consider a face-centered cubic lattice. Assume the atoms are hard spheres with the surfaces of the nearest neighbors touching. Assume the effective radius of the atom is 2.37 Å. (*a*) Determine the volume density of atoms in the crystal. (*b*) Calculate the surface density of atoms in the ~~(110)~~ plane. (*c*) Determine the distance between nearest ~~(110)~~ planes. (*d*) Repeat parts (*b*) and (*c*) for the (111) plane.



fcc cubic lattice in 3D



top view of top face of fcc

From the top view, the diagonal of the cell is $d = r + 2r + r = 4r = \sqrt{a^2 + a^2} = \sqrt{2}\, a$.

Therefore, $a = 4r / \sqrt{2} = 4(2.37) / \sqrt{2} \Rightarrow$ $\mathbf{a = 6.7034}$ **Å**

a) From left figure above,

atoms/unit cell = 8 corners (1/8 atom/corner) + 6 faces (1/2 atoms/face)
= 1 + 3 = 4

atomic volume density = *avd* = 4 atoms/a^3 = 4/(6.703×10^{-10} m)^3 = 1.328 × 10^{28} atoms/m^3

$\Rightarrow$ **<u>*avd* = 1.328 × 10^{22} atoms/cm^3</u>**

b) The (1 1 1) plane is the diagonal plane going through the solid dots at the top left back corner to front left bottom corner to back right bottom corner of the unit cell which form an isosceles triangle.

atoms$_{(1\,1\,1)}$ = 3 corners (60/360 atoms/corner) + 3 faces (1/2 atom/face)
= 0.5 + 1.5 = 2

The base *b* of the isosceles triangle is $b = \sqrt{a^2 + a^2} = \sqrt{2}\, a$.

The height *h* of the isosceles triangle is $h = 0.5 b \tan 60° = 0.5(\sqrt{2}\, a)\sqrt{3} = \sqrt{2}\sqrt{3}\, a / 2$.

$A_{(1\,1\,1)} = 0.5(\text{base})\text{height} = 0.5(\sqrt{2}\, a)\sqrt{2}\sqrt{3}\, a / 2 = \sqrt{3}\, a^2 / 2$

$asd_{(1\,1\,1)}$ = # atoms$_{(1\,1\,1)}$ / $A_{(1\,1\,1)}$ = 2/(√3a^2/2) = 4/√3/(6.7×10^{-10})^2 = 5.1394 × 10^{18} atoms/m^2

$\Rightarrow$ **<u>$asd_{(1\,1\,1)}$ = 5.139 × 10^{14} atoms/cm^2</u>**

c) **Method 1** Use the Cartesian coordinates shown in the left figure above.

In the left figure above, the nearest adjacent (1 1 1) planes are:

plane 1 defined by the solid dots at the front left bottom (a, 0, 0), back right bottom (0, a, 0), & top left back (0, 0, a) corners of the unit cell, and

plane 2 defined by the circles centered on the front (a, a/2, a/2), right (a/2, a, a/2), & top (a/2, a/2, a) faces of the unit cell.

The equation of a plane passing through points (x_1, y_1, z_1), (x_2, y_2, z_2), and (x_3, y_3, z_3) is

$$\begin{vmatrix} y_2-y_1 & z_2-z_1 \\ y_3-y_1 & z_3-z_1 \end{vmatrix}(x-x_1)+\begin{vmatrix} z_2-z_1 & x_2-x_1 \\ z_3-z_1 & x_3-x_1 \end{vmatrix}(y-y_1)+\begin{vmatrix} x_2-x_1 & y_2-y_1 \\ x_3-x_1 & y_3-y_1 \end{vmatrix}(z-z_1)=0.$$

Plane 1 is $\begin{vmatrix} a-0 & 0-0 \\ 0-0 & a-0 \end{vmatrix}(x-a)+\begin{vmatrix} 0-0 & 0-a \\ a-0 & 0-a \end{vmatrix}(y-0)+\begin{vmatrix} 0-a & a-0 \\ 0-a & 0-0 \end{vmatrix}(z-0)=0$

$$a^2(x-a)+a^2y+a^2z=0$$

which yields $\underline{\boldsymbol{x+y+z-a=0}}$

Plane 2 is

$$\begin{vmatrix} a-a/2 & a/2-a/2 \\ a/2-a/2 & a-a/2 \end{vmatrix}(x-a)+\begin{vmatrix} a/2-a/2 & a/2-a \\ a-a/2 & a/2-a \end{vmatrix}(y-a/2)+\begin{vmatrix} a/2-a & a-a/2 \\ a/2-a & a/2-a/2 \end{vmatrix}(z-a/2)=0$$

$$\begin{vmatrix} a/2 & 0 \\ 0 & a/2 \end{vmatrix}(x-a)+\begin{vmatrix} 0 & -a/2 \\ a/2 & -a/2 \end{vmatrix}(y-a/2)+\begin{vmatrix} -a/2 & a/2 \\ -a/2 & 0 \end{vmatrix}(z-a/2)=0$$

$$\frac{a^2}{4}(x-a)+\frac{a^2}{4}(y-a/2)+\frac{a^2}{4}(z-a/2)=0$$

which yields $\underline{\boldsymbol{x+y+z-2a=0}}$

The equation for the distance d between the parallel planes $C_1x + C_2y + C_3z - d_1 = 0$ and $C_1x + C_2y + C_3z - d_2 = 0$ is

$$d=\frac{|d_2-d_1|}{\sqrt{C_1^2+C_2^2+C_3^2}}$$ where we have $C_1 = C_2 = C_3 = 1$, d_1 = -a, and d_2 = -2a.

Therefore, the distance between adjacent (1 1 1) planes is

$$d_{(1\,1\,1)}=\frac{|-2a+a|}{\sqrt{1+1+1}}=\frac{a}{\sqrt{3}}=\frac{6.7034}{\sqrt{3}} \Rightarrow \underline{\boldsymbol{d_{(1\,1\,1)}=3.87\text{ Å}}}.$$

Method 2 Per https://en.wikipedia.org/wiki/Miller_index, the distance between planes defined by Miller indices (h k l) for **cubic lattices** w/ lattice constant a is

$$d_{(h\,k\,l)}=\frac{a}{\sqrt{h^2+k^2+l^2}}.\ \text{So, } d_{(1\,1\,1)}=\frac{a}{\sqrt{1^2+1^2+1^2}}=\frac{a}{\sqrt{3}}=\frac{6.7034}{\sqrt{3}} \Rightarrow \underline{\boldsymbol{d_{(1\,1\,1)}=3.87\text{ Å}}}.$$