Homework 2

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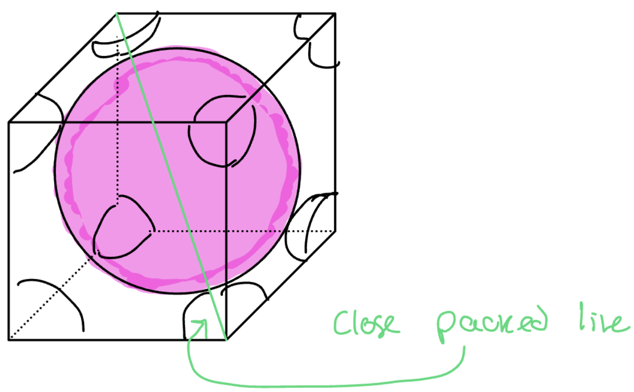
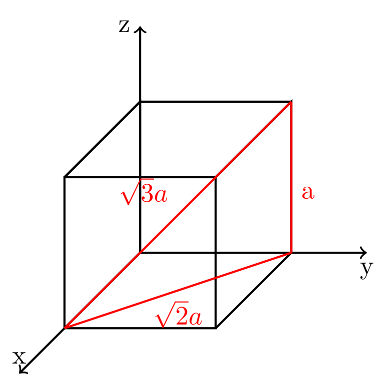
September 10, 2024

1 Unit Cell Volume

For BCC the close packed direction is [111]. This can be visualized like this



Then looking at the geometry



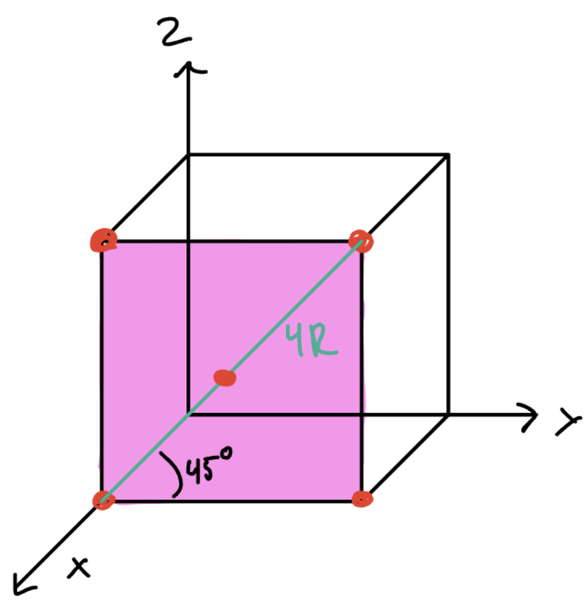
Along this direction the atoms are touching, so the close packed direction also has 4 atomic radii

$$
\begin{aligned}
4r &= \sqrt{3}a \\
a &= \frac{4r}{\sqrt{3}}
\end{aligned}
$$

$$
\begin{aligned}
V &= a^3 \\
&= \left(\frac{4r}{\sqrt{3}}\right)^3 \\
&= \left[0.1249\text{nm} \times \frac{4}{\sqrt{3}}\right]^3 \\
&= 0.02400\text{nm}^3
\end{aligned}
$$

2 Planar Density

(100) Plane



From this we see the relationship between the lattice parameter and the atomic radius

$$
\begin{aligned}
4r\cos(45^o) &= a \\
a &= 2\sqrt{2}r
\end{aligned}
$$

And the area of the plane is

$$
\begin{aligned}
A &= a^2 \\
&= (2\sqrt{2}r)^2 \\
&= 8r^2 \\
&= 0.1242 \text{ nm}^2
\end{aligned}
$$

So the planar density is

$$\frac{2}{0.1242} = 16 \text{ nm}^{-2}$$

(110) Plane

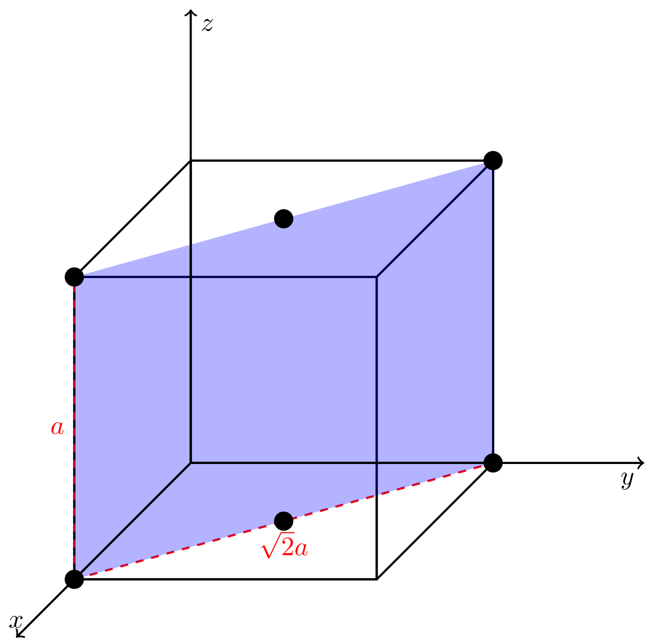


Figure 1: (110) Plane in an FCC Unit Cell

The same relationship between a and r, $a = 2\sqrt{2} \times r$, still holds. There are 2 half atoms and 4 quarter atoms in the plane, so there are two atoms in the plane. The diagonal of unit cell is $\sqrt{a}$, so

$$\begin{aligned} A &= a \times a\sqrt{2} \\ &= 8\sqrt{2}r^2 \\ &= 0.1756\text{nm}^2 \end{aligned}$$

So the planar density is

$$\frac{2}{0.1756} = 11.4\text{nm}^{-2}$$

(111) Plane

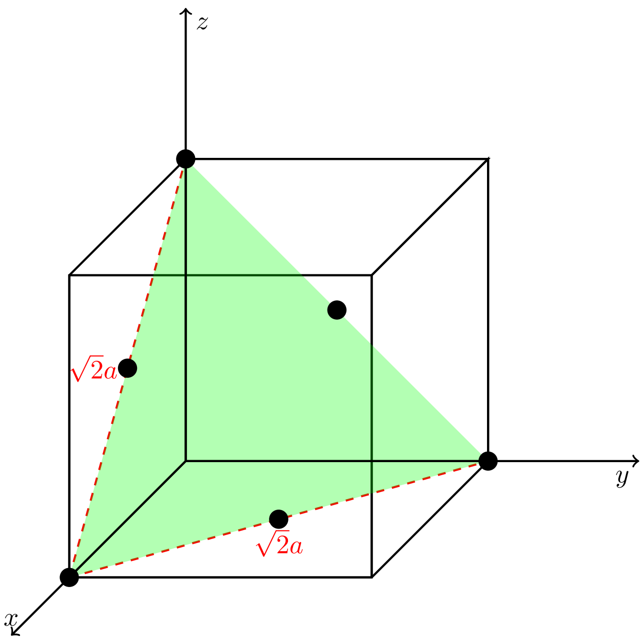


Figure 2: (111) Plane in an FCC Unit Cell

The same relationship between r and a still holds. There are 3 half atoms and 3 1/6th atoms, so two atoms in the plane. For the area of the plane we can use the

$$\begin{aligned} A &= \frac{\sqrt{3}}{4}a^2 \\ &= \frac{\sqrt{3}}{4}(\sqrt{2}(2\sqrt{2}r))^2 \\ &= 4\sqrt{3}r^2 \\ &= 0.1075 \text{ nm}^2 \end{aligned}$$

So the planar density is

$$\frac{2}{0.1075} = 18.6 \text{ nm}^{-2}$$

3 Theoretical Density

From Table 12.3

Ion	Radius (nm)
K^+	0.138
I^-	0.220

Which gives

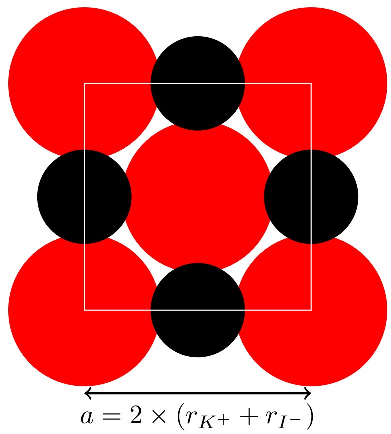
$$\frac{r_{K^+}}{r_{I^-}} = \frac{0.138}{0.220} = 0.627$$

So this is predicted to be 6 coordinated, which is a rock salt structure. The theoretical density is

$$\rho = \frac{n' \times (A_c + A_n)}{V_c \times N_A}$$

(eqn 12.1 in the book)

n' in this case is 4 because both of the ions are packed like FCC, which is 4 atoms per unit cell. A_c is 39.098 in this case, and A_n is 126.904. V_c is the volume of the unit cell. Looking at just one of the faces of the unit cell



So the volume of the unit cell is

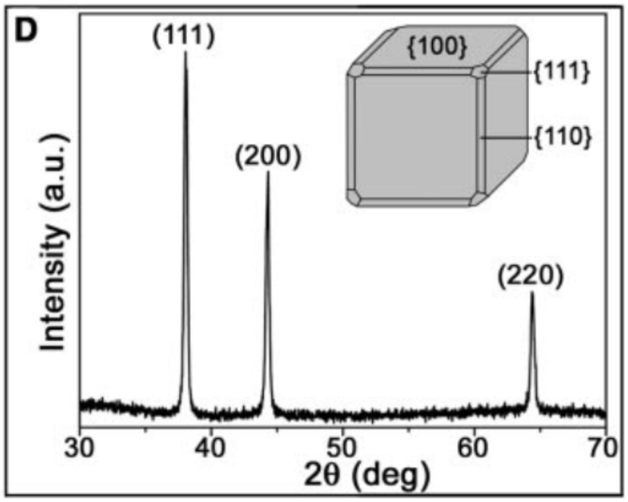
$$\begin{aligned} V_c &= a^3 \\ &= (2 \times (0.138 + 0.220))^3 \\ &= 0.367 \text{ nm}^3 \times \left(\frac{1 \text{ cm}}{10^7 \text{ nm}}\right)^3 \qquad = 3.67 \times 10^{-23} \text{ cm}^3 \end{aligned}$$

So, finally, the density is

$$\begin{aligned} \rho &= \frac{4 \times (39.098 + 126.904)}{3.67 \times 10^{-23} \times 6.022 \times 10^{23}} \\ &= 3.01 \text{ g/cm}^3 \end{aligned}$$

4 X-ray Diffraction

Replicating the figure Here



The authors say on the second page that they calculated the lattice constant, a, to be 4.088 Angstromg. Looking at the (111) plane, *assuming* that $n = 1$, and reading the angle off the graph as $2\theta = 38^o$,

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} = \frac{0.4088 \text{ nm}}{\sqrt{3}} = 0.2834 \text{ nm}$$

$$\lambda = \frac{2 \cdot d \cdot \sin(\theta)}{n}$$
$$\lambda = \frac{2 \cdot 0.2834 \cdot \sin(\frac{38^o}{2})}{1}$$
$$\lambda = 0.154 \text{ nm}$$

5 X-ray Diffraction cont.

a.

Rearranging the Bragg equation and slapping in known values

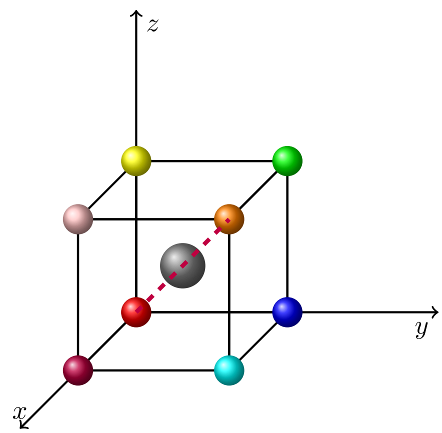
$$\begin{aligned} d &= \frac{n \cdot \lambda}{2 \cdot \sin(\theta)} \\ &= \frac{1 \cdot 0.0711}{2 \cdot \sin(\frac{20^o}{2})} \\ &= 0.152 \text{ nm} \end{aligned}$$

b.

We can use the d-spacing to find the lattice constant, and then that to find the radius

$$
\begin{aligned}
d &= \frac{a}{\sqrt{h^2+k^2+l^2}} \\
&= \frac{a}{\sqrt{3^2+2^2+1^2}} \\
&= \frac{a}{\sqrt{14}} \\
a &= d \cdot \sqrt{14} \\
&= 0.152 \cdot \sqrt{14} \\
&= 0.5698 \text{ nm}
\end{aligned}
$$

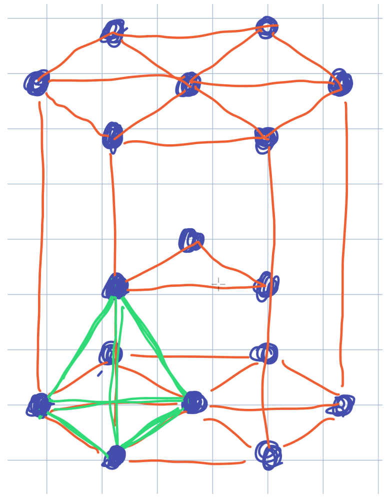
Then looking at a BCC unit cell



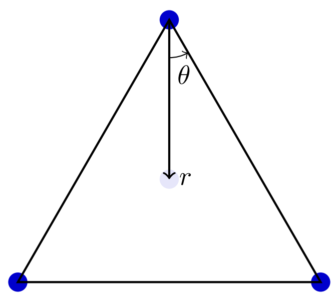
The close packed direction is [111] (shown above in dashed line) and gives us the relationship

$$
\begin{aligned}
4r &= \sqrt{3} \cdot a \\
r &= \frac{\sqrt{3} \cdot a}{4} \\
&= \frac{\sqrt{3} \cdot 0.5698 \text{ nm}}{4} \\
&= 0.247 \text{ nm}
\end{aligned}
$$

6 HCP System



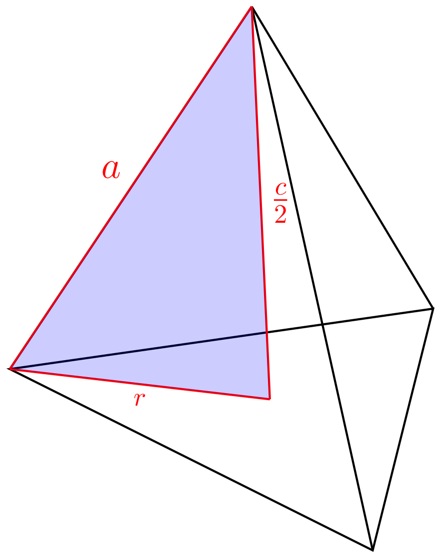
Looking at my little ipad sketch, you can see theres a fun tetrahedron I outlined in green. The tetrahedron has a height of $c/2$ and a base side length of a. The radius from the points of the base of the tetrahedron to the edges, r, can be visualized Here



The angle θ is 30^o, so

$$\frac{a}{2} = r\cos(30^o)$$
$$r = \frac{a}{\sqrt{3}}$$

Delicious. Now Looking at another visualization of the tetrahedron



$$a^2 = \left(\frac{c}{2}\right)^2 + r^2$$
$$a^2 = \left(\frac{a}{\sqrt{3}}\right)^2 + \left(\frac{c}{2}\right)^2$$
$$a^2 = \frac{a^2}{3} + \frac{c^2}{4}$$
$$\frac{2a^2}{3} = \frac{c^2}{4}$$
$$\frac{c^2}{a^2} = \frac{8}{3}$$
$$\frac{c}{a} = \sqrt{\frac{8}{3}}$$
$$\approx 1.633$$

6.1 b.

in each cell there are 12 1/6th atoms, 3 whole atoms, and 2 half atoms. So the number of atoms per cell is 6. The cell is close paced on the hexagon edges, so $2r = a$. We also know that $c = \sqrt{\frac{8}{3}} \cdot a$.

The volume of the atoms is

$$V_{atoms} = 6 \times \frac{4}{3}\pi r^3$$

the volume of the unit cell is

$$V_{cell} = c \times \left[\frac{3\sqrt{3}}{2}a^2\right]$$
$$= \left(2\sqrt{\frac{8}{3}}r\right)\left[\frac{3\sqrt{3}}{2}(2r)^2\right]$$

So the pacing factor is

$$
\begin{aligned}
APF &= \frac{V_{atoms}}{V_{cell}} \\
&= \frac{6 \times \frac{4}{3}\pi r^3}{\left(2\sqrt{\frac{8}{3}}r\right)\left[\frac{3\sqrt{3}}{2}(2r)^2\right]} \\
&= \frac{\pi}{3\sqrt{2}} \\
&\approx 0.74
\end{aligned}
$$

And just to quick run through the math on the FCC in case I needed to show they're EXACTLY the same

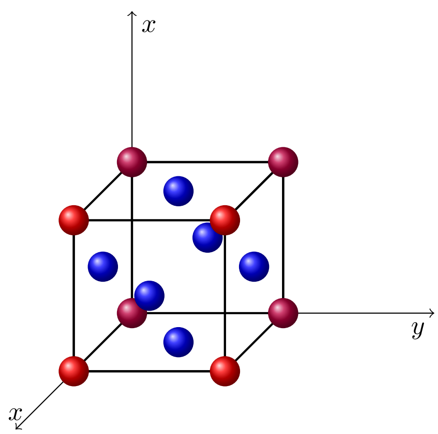


Figure 3: FCC Unit Cell with Blue Face-Centered Atoms and Red Corner Atoms

Of course the FCC has 4 atoms per cell, and the volume of the atoms is

$$V_{atoms} = 4 \times \frac{4}{3}\pi r^3$$

We also know, in general, FCC has the relationship

$$4r = \sqrt{2} \cdot a$$

So the volume of the unit cell is

$$V_{cell} = a^3 = \left(\frac{4r}{\sqrt{2}}\right)^3$$

So the packing factor is

$$
\begin{aligned}
APF &= \frac{V_{atoms}}{V_{cell}} \\
&= \frac{4 \times \frac{4}{3}\pi r^3}{\left(\frac{4r}{\sqrt{2}}\right)^3} \\
&= \frac{16\pi r^3}{\frac{32}{\sqrt{2}} r^3} \\
&= \frac{2\sqrt{2}}{12}\pi \\
&= \frac{\pi}{3\sqrt{2}} \\
&\approx 0.74
\end{aligned}
$$