Donald P. Shiley School of Engineering
EGR 221 Materials Science
Assignment 2, Fall 2015

1 a) Why is “helium” called helium? When and where was it first detected?
1 b) Why is “titanium” called titanium? When and where was it first detected? "GOOGLE"

2) Show for the body-centered cubic crystal structure that the unit cell edge length a and the atomic radius R are related through a =4R/ $(3)^{1/2}$

3) Show that the atomic packing factor for HCP is 0.74.

4) Iron has a BCC crystal structure, an atomic radius of 0.124 nm, and an atomic weight of 55.85 g/mol. Determine the theoretical density. How does it compare with the experimentally determined value of 7.87g/cm^3? The theoretical density is close to experimental, but measurably different. What conclusion do you reach from this?

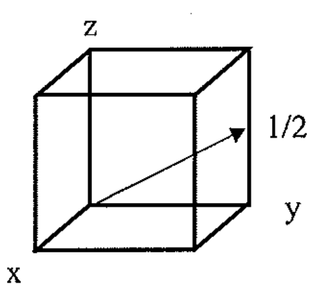
5) What are the point coordinates for all atoms in the following crystal structures’ unit cells (don’t forget to include appropriate sketches):

a) FCC
b) BCC

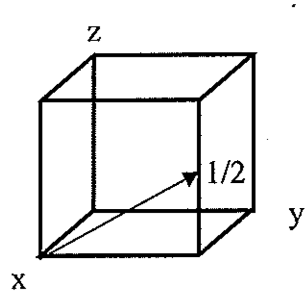
6) Within a cubic unit cell, sketch the following directions:

(a) $[1\,\bar{1}\,0]$, (b) [1 2 1], (c) [0 2 1], (d) $[\,0\,\bar{1}\,0]$

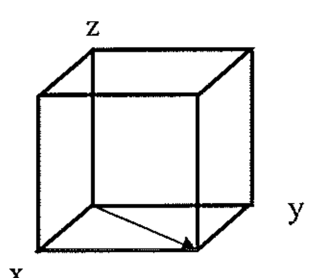
7) Determine the indices for the following directions in the cubic unit cell (for 3D visualization, assume both ends of the arrows are on the edge of the unit cell shown):



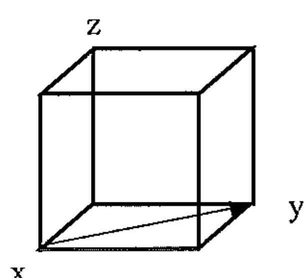
(a)



(b)



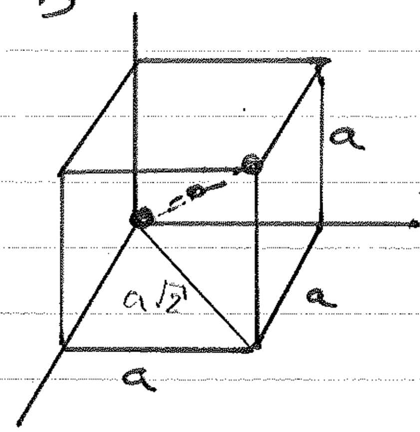
(c)



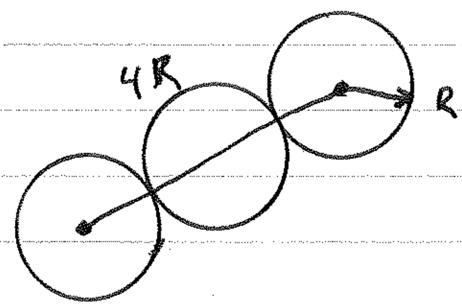
(d)

Show $a = \frac{4R}{\sqrt{3}}$ for BCC

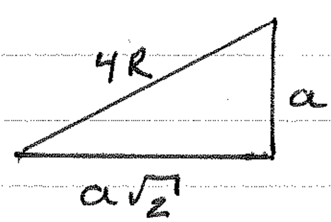
SOL'N: (INCLUDE SKETCH!)



For BCC, atoms 'touch' along the cube's diagonal.



Diagonal distance: 4R



$$4R = \sqrt{(a\sqrt{2})^2 + a^2}$$

$$4R = \sqrt{3a^2}$$

$$R = \frac{\sqrt{3}\,a}{4}$$

$$a = \frac{4R}{\sqrt{3}} = \frac{4\sqrt{3}\,R}{3}$$

QED

Show that the atomic packing factor for HCP is 0.74.

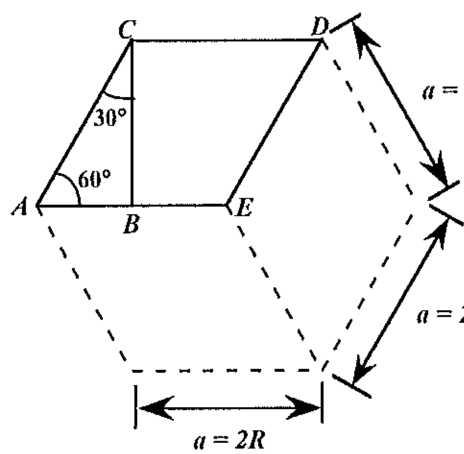
Assumptions: none required, this is pure math.

<u>Solution</u>

The APF is just the total sphere volume-unit cell volume ratio. For HCP, there are the equivalent of six spheres per unit cell, and thus

$$V_S = 6\left(\frac{4\pi R^3}{3}\right) = 8\pi R^3$$

Now, the unit cell volume is just the product of the base area times the cell height, c. This base area is just three times the area of the parallelepiped $ACDE$ shown below.



The area of $ACDE$ is just the length of $\overline{CD}$ times the height $\overline{BC}$. But $\overline{CD}$ is just a or $2R$, and

$$\overline{BC} = 2R\cos(30°) = \frac{2R\sqrt{3}}{2}$$

Thus, the base area is just

$$\text{AREA} = (3)(\overline{CD})(\overline{BC}) = (3)(2R)\left(\frac{2R\sqrt{3}}{2}\right) = 6R^2\sqrt{3}$$

and since $c = 1.633a = 2R(1.633)$

$$V_C = (\text{AREA})(c) = 6R^2c\sqrt{3}$$

$$= \left(6R^2\sqrt{3}\right)(2)(1.633)R = 12\sqrt{3}\,(1.633)\,R^3$$

Thus,

$$\text{APF} = \frac{V_S}{V_C} = \frac{8\pi R^3}{12\sqrt{3}\,(1.633)\,R^3} = 0.74 \qquad \text{QED}$$

Given: Fe is BCC (unless very hot)

$R = 0.124$ nm

atomic wt: 55.85 g/mole $= A_{Fe}$

Avogadro's #: 6.02×10^{23} mol^{-1} $= N_A$

Experimental density: 7.87 g/cc

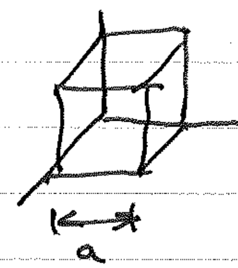
Find Theoretical density, ρ_{TH}

Sol'n: Consider 1 unit cell.

For BCC, there are 2 atom/unit cell

($\frac{1}{8} * 8$ - corner atoms + 1 center atom = 2 atoms)

$$a = \frac{4R}{\sqrt{3}}$$



(see Problem above)

Using units (our friends):

$$\rho_{TH} = \left[\frac{55.85\,g}{mole}\right] \cdot \left[\frac{?\ mole}{unit\,cell}\right] \cdot \left[\frac{1}{volume\ of\ 1\ unit\,cell}\right] \Rightarrow \frac{g}{cc}$$

If there are 2 atoms/unit cell, there are:

$$\frac{2\ atom/unit\,cell}{N_A\ atoms/mole} = \left[\frac{2}{6.02 \times 10^{23}}\ \frac{mole}{unit\,cell}\right]$$

$$\text{Volume of 1 unit cell} = a^3 = \left(\frac{4R}{\sqrt{3}}\right)^3$$

$$\rho_{TH} = \left[\frac{55.85g}{\cancel{mole}}\right] \cdot \left[\frac{2}{6.02 \times 10^{23}} \frac{\cancel{mole}}{\text{unit cell}}\right] \cdot \left[\frac{1}{\left(\frac{4R}{\sqrt{3}}\right)^3}\right]$$

$$R = 0.124 \text{ nm} = 0.124 \times 10^{-9} \text{ m} \quad \text{(given)}$$
$$= 12.4 \times 10^{-9} \text{ cm}$$

$$\rho_{TH} = 7.90 \text{ g/cc}$$

$$\% \text{ Diff}: \quad \frac{7.90 - 7.87}{7.87} = 0.4\% \text{ differce.}$$

The measured density is slightly less than theoretical indicating there may be some small "void-like" volume in real iron.

What are the point coordinates (aka locations, positions) of all atoms in FCC & BCC?

The location of corner atoms is the same for FCC & BCC.

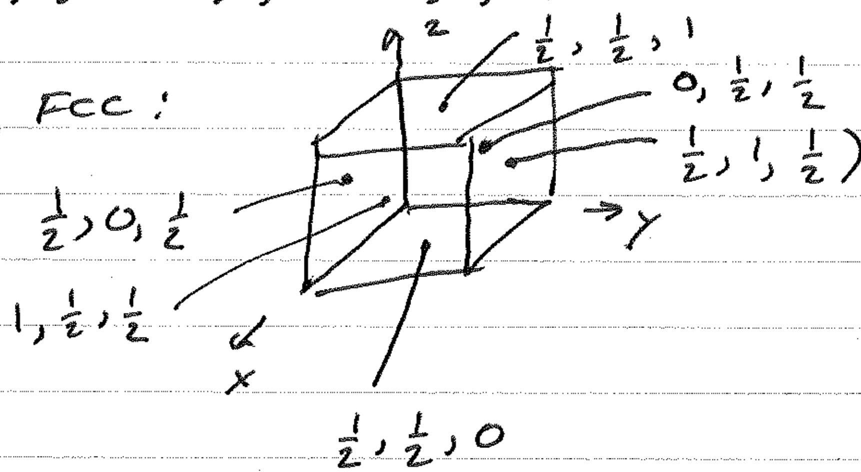
Corner atoms in x-y plane:

$(0,0,0)\ (1,0,0)\ (1,1,0)\ (0,1,0)$

Corner atoms on "top" of cube:

$(0,0,1)\ (1,0,1)\ (1,1,1)\ (0,1,1)$

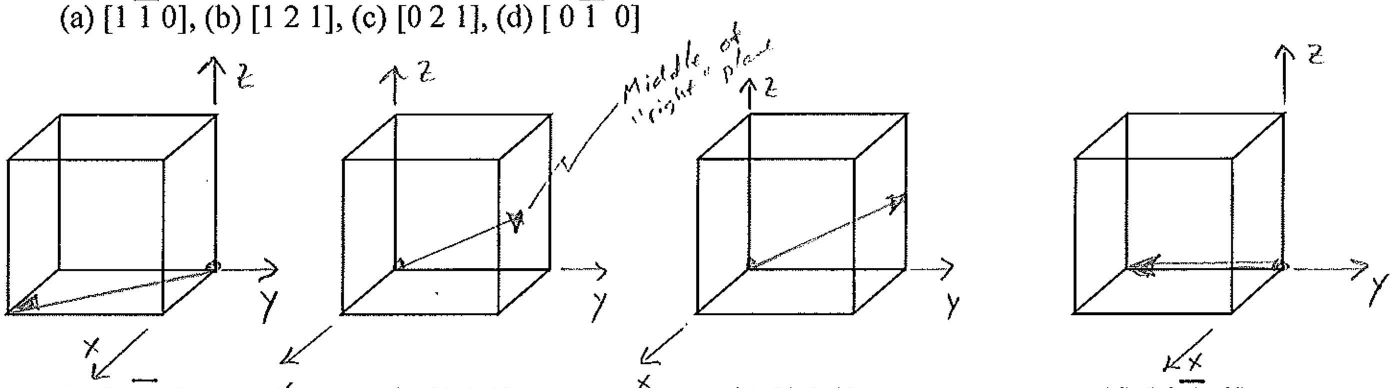
6 face atoms, FCC:



Center atom in BCC: $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

6) Within a cubic unit cell, sketch the following directions:

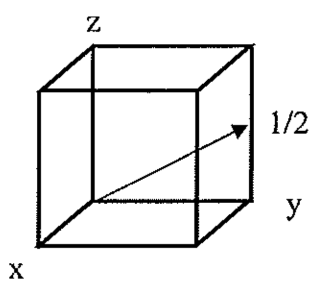
(a) $[1\bar{1}0]$, (b) $[1\,2\,1]$, (c) $[0\,2\,1]$, (d) $[0\bar{1}0]$



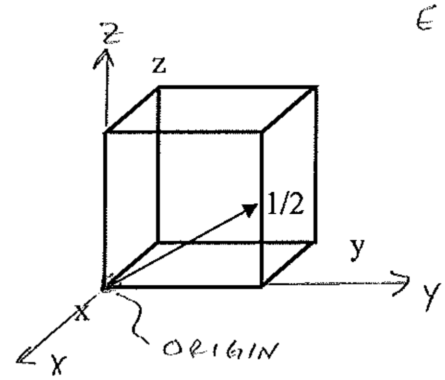
(a) $[1\bar{1}0]$ (b) $[1\,2\,1]$ (c) $[0\,2\,1]$ (d) $[0\bar{1}0]$

PT: 1, -1, 0 ½, 1, ½ 0, 1, ½ 0, -1, 0

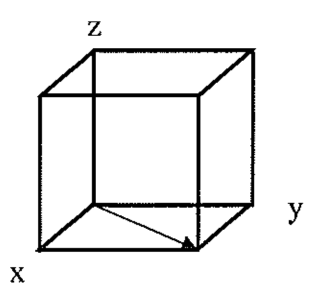
7) Determine the indices for the following directions in the cubic unit cell (for 3D visualization, assume both ends of the arrows are on the edge of the unit cell shown):



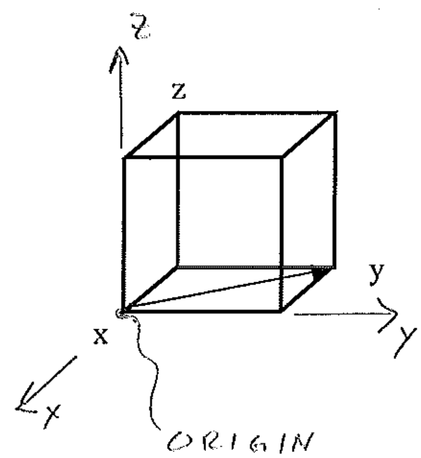
END PT:
0, 1, $\frac{1}{2}$ (x2)
[0 2 1]



END PT
0, 1, $\frac{1}{2}$ (x2)
[0 2 1]



END PT:
1, 1, 0
[1 1 0]



END PT:
-1, 1, 0
$[\bar{1}\,1\,0]$