

ENGR 240 Science of Materials – Spring 2001-
Homework Assignment 4 Solutions
15 points

1. [2 points] Calculate the atomic packing factor (APF) for the bcc unit cell. Use equation 3.2:

$$APF = \frac{\text{total volume of spherical atoms in a unit cell}}{\text{total unit cell volume}} = \frac{V_s}{V_c}$$

The bcc structure has 2 atoms per unit cell.

$$APF = \frac{V_s}{V_c} = \frac{2 \times \left(\frac{4}{3} \pi R^3 \right)}{\left(\frac{4R}{\sqrt{3}} \right)^3} = 0.680$$

2. [3 points] Nickel has the fcc structure and a lattice parameter of $a = 0.3517 \text{ nm}$.
- Determine the atomic radius in nm.
 - Determine the atomic volume Ω in nm^3 (assume a spherical atom shape).
 - Determine the density in g/cm^3 and compare this answer to the Ni density value given in the table at the front of your textbook.

a. $R = a/(2\sqrt{2}) = 0.124 \text{ nm}$

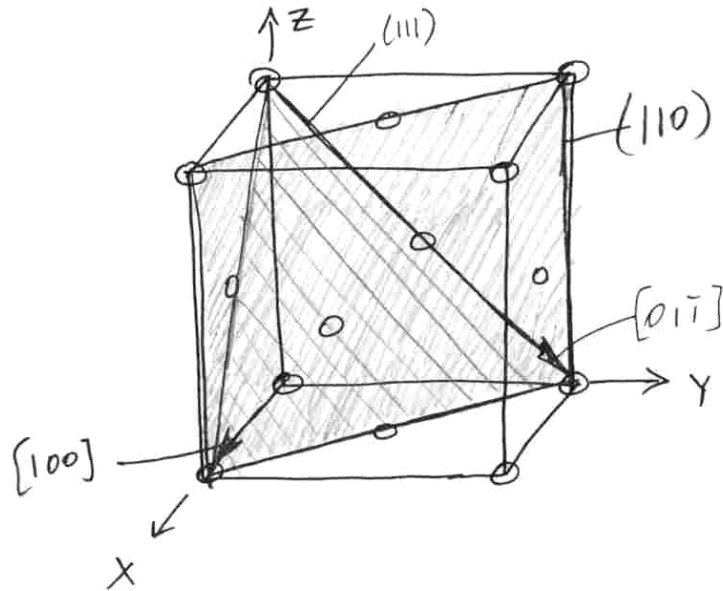
b. Assuming a spherical atoms, $\Omega = 4\pi R^3/3 = .000805 \text{ nm}^3 = 8.05 \times 10^{-3} \text{ nm}^3$

c. Use Equation 3.5 on page 37:

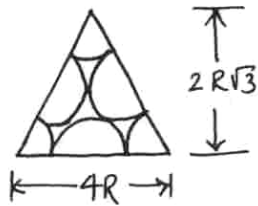
$$\rho = \frac{nA}{V_c N_A} = \frac{4 \text{ atoms/cell} \cdot 58.693 \text{ g/mol}}{(0.3517 \text{ nm})^3 \cdot (6.023 \times 10^{23} \text{ atoms/mol})} = 8.96 \times 10^{-21} \text{ g/nm}^3 = 8.96 \text{ g/cm}^3$$

Book value for nickel density is 8.90 g/cm^3 , so the values are very close (hard sphere model is pretty good).

3. [4 points] Planar and linear atomic densities in fcc structure:



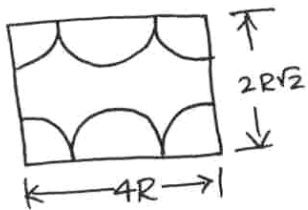
(a) (111) PLANAR DENSITY



$$3 \cdot \frac{1}{6} + 3 \cdot \frac{1}{2} = 2 \text{ ATOMS}$$

$$PD = \frac{\text{AREA OF ATOMS}}{\text{AREA OF PLANE}} = \frac{2 \text{ ATOMS} \cdot \pi R^2}{4R^2 \sqrt{3}} = \underline{\underline{0.907}}$$

(b) (110) PLANAR DENSITY



$$PD = \frac{2 \text{ ATOMS} \cdot \pi R^2}{8R^2 \sqrt{2}} = \underline{\underline{0.555}}$$

(c) [011] LINEAR DENSITY

$$LD = \frac{\text{LINE LENGTH OF ATOMS}}{\text{TOTAL LINE LENGTH}} = \frac{4R}{a\sqrt{2}} = \frac{4R}{4R} = \underline{\underline{1}}$$

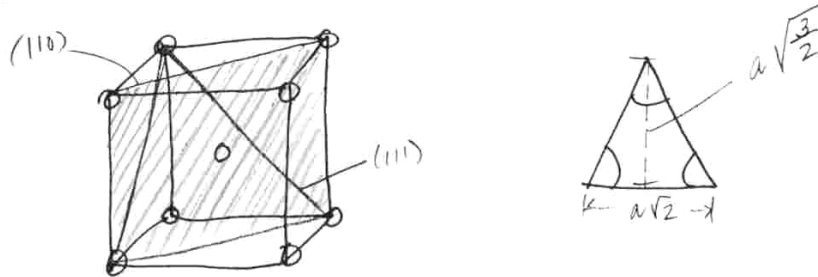
(d) [100] LINEAR DENSITY

$$LD = \frac{2R}{a} = \frac{2R}{2R\sqrt{2}} = \frac{1}{\sqrt{2}} = \underline{\underline{0.707}}$$

4. [2points] Planar densities in bcc structure.

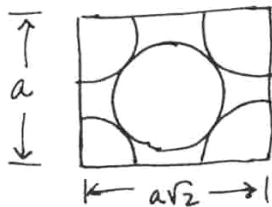
(a) [$\frac{1}{2}$ POINT] (111)

* ONLY COUNT ATOMS IF THE PLANE
PASSES THROUGH THE CENTER *



$$PD = \frac{\frac{1}{2} \text{ ATOM} \cdot \pi R^2}{\frac{1}{2} \cdot a\sqrt{2} \cdot a\sqrt{\frac{3}{2}}} = \frac{\pi R^2}{a^2\sqrt{3}} = \frac{2\pi R^2}{16R^2\sqrt{3}} = \underline{\underline{0.340}}$$

(b) [$\frac{1}{2}$ POINT] (110)



$$PD = \frac{2 \text{ ATOMS} \cdot \pi R^2}{a^2\sqrt{2}} = \frac{2\pi R^2}{\left(\frac{4R}{\sqrt{3}}\right)^2\sqrt{2}} = \frac{2\pi R^2}{\frac{16R^2}{3}\sqrt{2}} = \underline{\underline{0.833}}$$

5. [3 points] Callister Problem 3.56 For each peak, in order to compute the interplanar spacing and the lattice parameter we must employ Equations (3.10) and (3.9), respectively. For the first peak which occurs at 45.0°

$$d_{110} = \frac{nl}{2 \sin \theta} = \frac{(1)(0.1542 \text{ nm})}{(2) \left(\sin \frac{45.0^\circ}{2} \right)} = 0.2015 \text{ nm}$$

And

$$\begin{aligned} a &= d_{hkl} \sqrt{(h)^2 + (k)^2 + (l)^2} = d_{110} \sqrt{(1)^2 + (1)^2 + (0)^2} \\ &= (0.2015 \text{ nm})\sqrt{2} = 0.2850 \text{ nm} \end{aligned}$$

Similar computations are made for the other peaks which results are tabulated below:

<u>Peak Index</u>	<u>2θ</u>	<u>$d_{hkl}(\text{nm})$</u>	<u>$a(\text{nm})$</u>
200	65.1	0.1433	0.2866
211	82.8	0.1166	0.2856

6. [1 point] No, single crystal properties generally vary with crystallographic directions. For example, aluminum (fcc) is stiffer in the $[111]$ than in the $[100]$ direction. See Table 3.3 on page 53 of Callister.