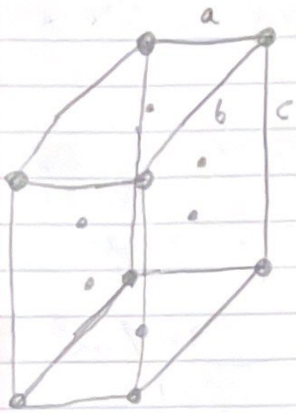
HW#3

1) U has FCC w/ $a = 285.37\ pm$, $b = 586.95\ pm$, $c = 495.85\ pm$, $\alpha = \beta = \gamma = 90°$

$R = 138\ pm$



a) $APF = \dfrac{\forall_{filled}}{\forall_{cell}} = \boxed{0.54737}$

$\forall_{cell} = abc = 8.04468e{-23}\ cc$

$\forall_{filled} = n_{atoms} \forall_{atom} = 4.40338e{-23}\ cc$

$\hookrightarrow n_{atoms} = 8\left(\frac{1}{8}\right) + 6\left(\frac{1}{2}\right) = 4$ atoms / unit cell

$\hookrightarrow \forall_{atom} = \frac{4}{3}\pi R^3 = \frac{4}{3}\pi(138\ pm)^3 = 1.10084e{-23}\ cc$

b) $\rho = \dfrac{\text{mass in a cell}}{\forall_{cell}} = \dfrac{1}{\forall_{cell}} \cdot m_u \cdot \dfrac{1.66054e{-24}g}{u\ (\text{dalton})} \cdot n_{atoms}$

$\rho = \dfrac{1}{\forall_{cell}}(238.02891\ u)\left(\dfrac{1.66054e{-24}g}{u}\right)4 = \boxed{19.65\ g/cc}$ $\approx 19.1\ g/cm^3$ for accepted val

HW #3 - cont

2) we know $2d\sin\theta = n\lambda$ & $a = d\sqrt{h^2+k^2+l^2}$

$$\Rightarrow 2\left(\frac{a}{\sqrt{h^2+k^2+l^2}}\right)\sin\theta = n\lambda \Rightarrow \frac{2a}{n\lambda}\sin\theta = \sqrt{h^2+k^2+l^2} \Rightarrow \sin^2\theta \propto h^2+k^2+l^2$$

knowing that $\sin^2\theta \propto h^2+k^2+l^2$ allows us to compare $\sin^2\theta$ for the given peaks & θs to the known planes of BCC & FCC

$\star \rightarrow (x \equiv \sqrt{h^2+k^2+l^2}) \leftarrow \star$

BCC

index	$\|x\|^2$	$\|x\|^2/\min(\|x\|^2)$
(1 1 0)	2	1
(2 0 0)	4	2
(2 1 1)	6	3

FCC

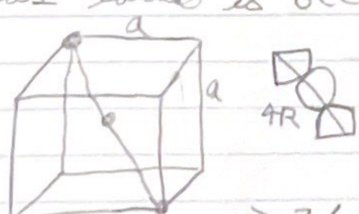
index	$\|x\|^2$	$\|x\|^2/\min(\|x\|^2)$
(1 1 1)	3	1
(2 0 0)	4	$1.\bar{3}$
(2 2 0)	8	$2.\bar{6}$

compare to the given peaks $\Rightarrow$

Peak	2θ	$\sin^2\theta$	$\sin^2\theta/\min(\sin^2\theta)$
1	18.27°	0.0252	1
2	25.96°	0.0504	2.0016
3	31.92°	0.0756	3.0000

a) $\boxed{\text{BCC}}$ b) as $|x|^2$ for the known BCC planes is proportional to $\sin^2\theta$ for the given peaks (see above for math)

c) as lattice is BCC, use eq. 3.4, $a = \frac{4R}{\sqrt{3}}$



& $a = d\sqrt{h^2+k^2+l^2} \Rightarrow d = \frac{a}{x} = \frac{4R}{x\sqrt{3}}$

$$\Rightarrow 2\left(\frac{4R}{x\sqrt{3}}\right)\sin\theta = n\lambda \Rightarrow R = \frac{n\lambda x\sqrt{3}}{8\sin\theta}$$ w/ $\lambda = 0.0711$ nm, $n = 1$

peak #1

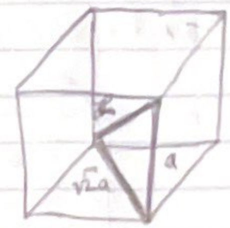
$$R = \frac{(1)(0.0711\text{ nm})(\sqrt{2})(\sqrt{3})}{8\sin(9.135°)} = \boxed{0.1371\text{ nm}}$$

which corresponds to $\boxed{\text{W}}$ in table 3.1

HW # 3 - cont.

3a) linear density of [111] direction in FCC.

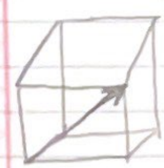
111 $\Rightarrow LD = \dfrac{n\ \text{atom}}{\mathcal{L}} = \dfrac{1}{2\sqrt{6}R} = \boxed{\dfrac{\sqrt{6}}{12R} = LD}$



$\mathcal{L}^2 = (\sqrt{2}a)^2 + (a)^2 = 3a^2$, w/ $a = 2R\sqrt{2}$, $\mathcal{L}^2 = 3(4R^2 2) = 24R^2$

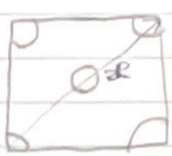
$\mathcal{L} = 2\sqrt{6}R$

b) linear density for [111] BCC.



$LD = \dfrac{\#\ \text{atoms}}{\mathcal{L}} = \dfrac{2}{4R} = \boxed{\dfrac{1}{2R} = LD}$

c) planar density of (100) planes in FCC.

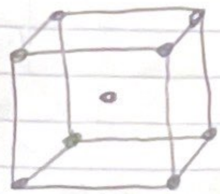


$PD = \dfrac{n\ \text{atoms}}{\text{area}} = \dfrac{2}{a^2} = \dfrac{2}{8R^2} = \boxed{\dfrac{1}{4R^2} = PD}$

$\mathcal{L} = a\sqrt{2}$, $\mathcal{L} = 4R \Rightarrow a = 2R\sqrt{2} \Rightarrow a^2 = 4R^2(2)$

HW #3 - cont

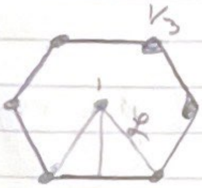
3d) Planar density for (100) plane in BCC



$$PD = \frac{n}{\text{area}} = \frac{1}{a^2} = \boxed{\frac{3}{16R^2} = PD}$$

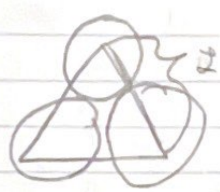
know $a = 4R/\sqrt{3} \Rightarrow a^2 = 16R^2/3$

e) Planar density of (0001) plane in HCP.



$$PD = \frac{n}{\text{area}} = \frac{3}{6R^2\sqrt{3}} = \boxed{\frac{\sqrt{3}}{6R^2} = PD}$$

area of regular n-gon $= nL^2 \sin\left(\frac{\pi}{n}\right)\cos\left(\frac{\pi}{n}\right)$



$L = 2R \therefore \text{area} = 6(2R)^2 \sin\left(\frac{\pi}{6}\right)\cos\left(\frac{\pi}{6}\right)$

$\text{area} = 24R^2\left(\frac{1}{2}\right)\left(\frac{\sqrt{3}}{2}\right) = 6R^2\sqrt{3}$

HW #3 - cont

4) Calculate # of vacancies / m^3 in gold @ 900°C (= 1173.15 K)
- Energy / vacancy formation = 0.98 eV / atom
- ρ = 18.63 g/cm³ & M = 196.9 g/mol

need $N = \frac{N_A \rho}{M} = \frac{(6.022e23 \frac{atoms}{mol})(18.63 \frac{g}{cc})(10^6 \frac{cm^3}{m^3})}{196.9 \text{ g/mol}}$

$N = 5.6978e28$ atoms / m³

next use Eq 4.1 to find N_v, number density of vacancies

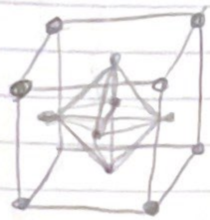
$$\Rightarrow N_v = N \exp\left(-\frac{Q_v}{kT}\right) = N \exp\left(\frac{-0.98 \frac{eV}{atom}}{(8.62e{-5} \frac{eV}{K})(1173 K)}\right)$$

$$\boxed{N_v = 3.51928e24 \ \frac{\text{vacancies}}{m^3}}$$

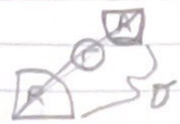
HW#3 - cont

5) FCC w/ radius R & interstitial impurities in cavities

a) find r of interstitial atom in octahedral cavity



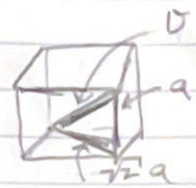
octahedral cavity in center of every unit cell, so look along cube diagonal, D



know $a = 2R\sqrt{2}$

also know $D^2 = (\sqrt{2}\,a)^2 + a^2 = 3a^2 = 3(4R^2(2)) = 24R^2$

$\hookrightarrow D = 2\sqrt{6}\,R$

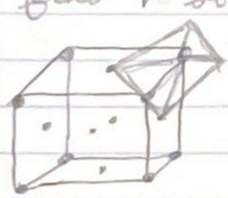


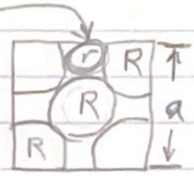
know $D = 2R + 2r$

$\Rightarrow 2R + 2r = 2\sqrt{6}\,R \Rightarrow R + r = \sqrt{6}\,R$

$\Rightarrow \boxed{r = R(\sqrt{6} - 1) \approx 1.449\,R}$ (a)

b) find r of interstitial atom in tetrahedral cavity





$a = 2R + 2r$

& $a = 2R\sqrt{2}$

$\Rightarrow 2R + 2r = 2R\sqrt{2} \Rightarrow R + r = R\sqrt{2} \Rightarrow r = R(\sqrt{2} - 1)$

$\boxed{r = R(\sqrt{2} - 1) \approx 0.414\,R}$ (b)

Sorry this one isn't as neat!
I've got a lot of work to do this week.