MAT E 201: Solution to Assignment #3

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Q1 A: $0,1,1-\frac{1}{2},1,0=-\frac{1}{2},0,1 \Rightarrow [\bar{1}02]$

$\Rightarrow h'=-1, k'=0, l'=2$

$h=\frac{1}{3}(2h'-k')=-\frac{2}{3}, \quad k=\frac{1}{3}(2k'-h')=\frac{1}{3}$

$i=-\frac{1}{3}(h'-k')=\frac{1}{3}, \quad l=l'=2$

$-\frac{2}{3}, \frac{1}{3}, \frac{1}{3}, 2 \mid \cdot 3 \Rightarrow [\bar{2}116]$

B: $1,0,0-1,1,1=0,-1,-1 \Rightarrow [0\bar{1}\bar{1}]$

$\Rightarrow h'=0, k'=-1, l'=-1$

$h=1/3, \quad k=-2/3, \quad i=1/3, \quad l=-1$

$\frac{1}{3}, -\frac{2}{3}, \frac{1}{3}, -1 \mid 3 \Rightarrow [\bar{1}2\bar{1}3]$

C: $0,0,0-0,-1,1=0,1,-1 \Rightarrow [01\bar{1}]$

$h'=0, k'=1, l'=1$

$h=-\frac{1}{3}, \quad k=\frac{2}{3}, \quad i=-\frac{1}{3}, \quad l=-1$

$-\frac{1}{3}, \frac{2}{3}, -\frac{1}{3}, -1 \Rightarrow [\bar{1}2\bar{1}\bar{3}]$

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Q2

$A: a_1 = 1,\ a_2 = -1,\ a_3 = \infty,\ c = \frac{1}{2}$

$\frac{1}{a_1} = 1,\ \frac{1}{a_2} = 1,\ \frac{1}{a_3} = 0,\ \frac{1}{c} = 2$

$\Rightarrow A(1\ \bar{1}\ 0\ 2)$

$B: a_1 = \infty,\ a_2 = 1,\ a_3 = -1,\ c = 1$

$\frac{1}{a_1} = 0,\ \frac{1}{a_2} = 1,\ \frac{1}{a_3} = -1,\ \frac{1}{c} = 1$

$\Rightarrow B(0\ 1\ \bar{1}\ 1)$

$C: a_1 = -1,\ a_2 = \frac{1}{2},\ a_3 = -1,\ c = \infty$

$\frac{1}{a_1} = -1,\ \frac{1}{a_2} = 2,\ \frac{1}{a_3} = -1,\ c = 0$

$\Rightarrow C(\bar{1}\ 2\ \bar{1}\ 0)$

Q3 Sn film $N(d_{100}) = 1.8 \cdot 10^6$ FCC Sn (100)

$d_{100} = ?$ $a_0 = 0.64912\,nm$ $h=1, k=0, l=0$

$$d_{hkl} = d_{100} = \frac{a_0}{\sqrt{h^2+k^2+l^2}} = \frac{6.4912 \cdot 10^{-8}\,cm}{\sqrt{1^2+0^2+0^2}}$$

$$d_{100} = 6.4912 \cdot 10^{-8}\,cm$$

$$N(d_{100}) = \frac{\delta}{d_{100}} \Rightarrow \delta = d_{100} \cdot N(d_{100})$$

$$\delta = 6.4912 \cdot 10^{-8} \cdot 1.8 \cdot 10^6 = 0.1168\,cm = 1.168\,mm$$

Q5

$r_{U^{4+}} = 0.97\text{Å}$ $\quad r_{O^{2-}} = 1.32\text{Å}$

Valence of U is +4; Valence of O is −2

In order to balance the charge there must be twice as many oxygen ions as uranium ions.

⇒ The fluorite structure will satisfy the requirem with:

U FCC position (4) ; O tetrahedral posi (8)

a) $\sqrt{3}\, a_0 = 4r_U + 4r_O = 4(0.97+1.32) = 9.16$

⇒ $a_0 = 5.2885\text{Å}$

b) $$\rho = \frac{4(238.03\ g/mol) + 8(16\ g/mol)}{(5.2885\cdot 10^{-8}\ cm)^3 \cdot 6.023\cdot 10^{23}\ at/mol}$$

$$\rho = 12.13\ g/cm^3$$

c) $$PF = \frac{(4\pi/3)\left[4(0.97)^3 + 8(1.32)^3\right]}{(5.2885)^3} = 0.624$$

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Q6 Al (311) $2\theta = 78.3°$ $\lambda = 0.15418\,nm$

$$\sin\theta = \frac{\lambda}{2d_{311}} \Rightarrow \quad d_{311} = \frac{a_0}{\sqrt{3^2+1^2+1^2}} = \frac{a_0}{\sqrt{11}}$$

$$a_0 = d_{311}\sqrt{11}$$

$$\sin\theta = \frac{\lambda}{2\cdot\frac{a_0}{\sqrt{11}}} = \frac{\lambda\sqrt{11}}{2a_0} \Rightarrow a_0 = \frac{\lambda\sqrt{11}}{2\sin\theta}$$

$$a_0 = \frac{0.15418\sqrt{11}}{2\sin\left(\frac{78.3}{2}\right)} = 0.40497\,nm$$