Material Science
Homework 1
Due Tuesday Oct 16, 2018

1. (3%)B: $[\bar{4}0\bar{3}]$;

   (3%)D: $[\bar{1}1\bar{1}]$;

   (4%)E: $\vec{E}=\overrightarrow{a_3}+\frac{1}{2}\overrightarrow{c}=\frac{1}{3}[\bar{1}\bar{1}20]+\frac{1}{2}[0001]=\frac{1}{6}[\bar{2}\bar{2}43]$

   註 1：因為方向的正負不同，因此差一個正負號則全錯

   註 2：HCP 的四軸表示法伴隨有長度的意味，因此前面的$\frac{1}{6}$加入更能表達單位晶胞內的方向

2. (a) Plane A is a $(32\bar{2})$ plane. (3%)

	x	y	z
Intercepts	$\frac{a}{3}$	$\frac{b}{2}$	$-\frac{c}{2}$
Intercepts in terms of a, b, and c	$\frac{1}{3}$	$\frac{1}{2}$	$-\frac{1}{2}$
Reciprocals of intercepts	3	2	-2
Reduction		(not necessary)	
Enclosure		$(32\bar{2})$	

   Plane B is a $(20\bar{2})$ plane. (2%)

	x	y	z
Intercepts	$-\frac{a}{2}$	∞b	$\frac{c}{2}$
Intercepts in terms of a, b, and c	$-\frac{1}{2}$	∞	$\frac{1}{2}$
Reciprocals of intercepts	-2	0	2

   $(\bar{2}02)$ or $(20\bar{2})$

   (b) Plane 1 is a (0 2 0) plane. (2%)

	x	y	z
Intercepts	∞a	$b/2$	∞c
Intercepts in terms of a, b, and c	∞	1/2	∞
Reciprocals of intercepts	0	2	0
Enclosure		(020)	

   Plane 2 is a $(2\bar{2}1)$ plane. (3%)

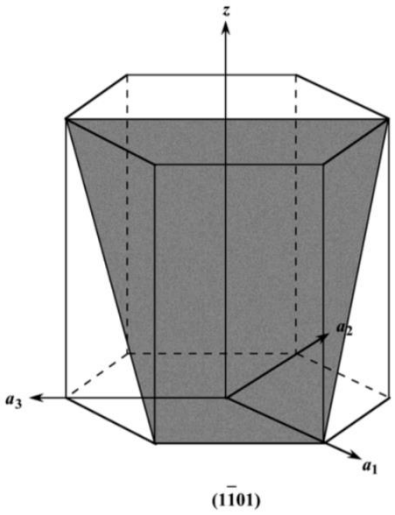
	x	y	z
Intercepts	$a/2$	$-b/2$	c
Intercepts in terms of a, b, and c	1/2	-1/2	1
Reciprocals of intercepts	2	-2	1
Enclosure		$(2\bar{2}1)$	

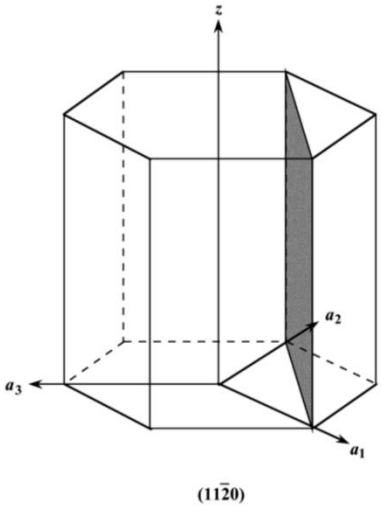
   註 1：(010)和(020)在 unit cell 表示的平面不完全相同，相似狀況以此類推，故會酌扣分數

   註 2：注意平面、平面族、方向、方向族的表示方法，不同表示方法意義不同

   註 3：在結晶結構中，截距不完全是指長度，截距是與各軸單位長度的比例

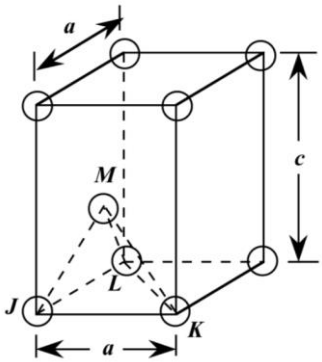
3.

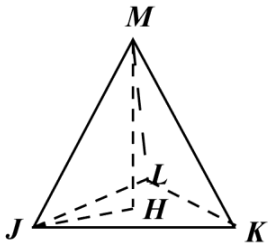




(5%) (5%)

4. A sketch of one-third of an ideal HCP unit cell is shown below.





$$\overline{MJ}^2 = \overline{MH}^2 + \overline{JH}^2$$

$$(a)^2 = \left(\frac{c}{2}\right)^2 + \left(\frac{2}{3}\times\frac{\sqrt{3}}{2}a\right)^2 \quad \rightarrow \quad \left(\frac{c}{a}\right)^2 = \frac{8}{3}$$

$$\frac{c}{a} = \sqrt{\frac{8}{3}} \approx 1.633 \quad (5\%)$$

$$\text{APF} = \frac{V_S}{V_C} = \frac{6\times\frac{4}{3}\pi R^3}{\left[6\times\frac{\sqrt{3}}{4}(2R)^2\right]\times\left(\sqrt{\frac{8}{3}}\times 2R\right)} = 0.74 \quad (5\%)$$

5. $$n = \frac{\rho V_C N_A}{A_{Sn}} = \frac{(7.30)(5.83\times10^{-8}cm)^2(3.18\times10^{-8}cm)N_A}{118.69} = 4\ \frac{atoms}{unit\ cell}$$

$$\text{APF} = \frac{V_S}{V_C} = \frac{n\times\frac{4}{3}\pi R^3}{a^2 c} = \frac{4\times\frac{4}{3}\pi(1.51\times10^{-8}cm)^3}{(5.83\times10^{-8}cm)^2(3.18\times10^{-8}cm)} = 0.534 = 53.4\% \quad (10\%)$$

6. In this case c=1.856a, for HCP, $a = 2R$, which means that $V_C = 6R^2c\sqrt{3} = 6R^2(1.856)(2R)\sqrt{3}$

The density equal to

$$\rho = \frac{nA_{Zn}}{V_C N_A} = \frac{nA_{Zn}}{(1.856)(12\sqrt{3})N_A R^3}$$

Solving R from above eq. lead to

$$R = \left[\frac{nA_{Zn}}{(1.856)(12\sqrt{3})\rho N_A}\right]^{\frac{1}{3}} = \left[\frac{6\times 65.41}{(1.856)(12\sqrt{3})(7.13)N_A}\right]^{\frac{1}{3}} = 0.133\,nm \quad (10\%)$$

7. (a) $\mathrm{LD}_{111} = \dfrac{number\ of\ atoms\ centered\ on\ [111]\ direction}{length\ of\ [111]\ direction}(in\ terms\ of\ R) = \dfrac{2\ atoms}{4R} = \dfrac{1}{2R}$ (5%)

$$\mathrm{PD}_{110} = \frac{number\ of\ atoms\ centered\ on\ (110)\ plane}{area\ of\ (110)\ plane}(in\ terms\ of\ R) = \frac{2\ atoms}{\frac{16\sqrt{2}}{3}R^2} = \frac{3}{8\sqrt{2}R^2} \quad (5\%)$$

(b) $\mathrm{LD}_{111} = \dfrac{1}{2R} = \dfrac{1}{2\times 0.137} = 3.650\,nm^{-1}$ (2.5%)

$$\mathrm{PD}_{110} = \frac{3}{8\sqrt{2}R^2} = \frac{3}{8\sqrt{2}(0.137)^2} = 14.128\,nm^{-2} \quad (2.5\%)$$

註：題目已經告知利用 R 證明線密度和面密度，故用百分比表示者不給分

8. (a) $V_C = \dfrac{nA_{Zr}}{\rho N_A} = \dfrac{6\times 91.22}{6.51\times N_A} = 1.396\times 10^{-22}\,cm^3/unit\ cell$ (10%)

(b) For HCP and c =1.593 a

$$V_C = 3\times a\times\frac{\sqrt{3}}{2}a\times c = \frac{3\sqrt{3}}{2}a^2c = \frac{3\sqrt{3}}{2}(1.593)a^3 = 1.396\times 10^{-22}\,cm^3/unit\ cel$$

Solving for a

$$a = \left[\frac{1.396\times 10^{-22}}{(\frac{3\sqrt{3}}{2})(1.593)}\right]^{\frac{1}{3}} = 0.323\,nm \quad (5\%)$$

$$c = 1.593\,a = 1.593\times 0.323 = 0.515nm \quad (5\%)$$

上面加總共 95 分，送 5 分，總分 100 分