

**Engineering Materials, Course No. 4202402, CCU ME**

**Mid-term Exam (I) 100.11.08.**

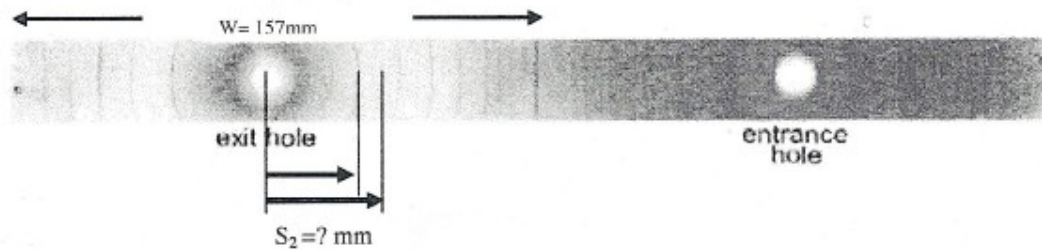
Lectured by: 敖仲寧

1. Total score: 120, 2. Close-book, 3. Using calculator is allowed, 4. Keep question sheets and return answering sheets.

1. (a) List all primary and secondary interatomic bonds (8%)  
(b) The net potential energy between two adjacent ions  $E_N$  may be expressed as  $E_N = -\frac{A}{r} + \frac{B}{r^n}$ , where  $r$  is the distance between two adjacent ions, and  $A, B$  are constants. Calculate the distance  $r_0$ , at which the potential energy  $E_N$  between two adjacent ions has a minimum value  $E_0$ . (Hint:  $r_0$  is expressed in terms of  $A, B$  and  $n$ .) (10%)
2. (a) List any 5 crystal systems and give for each crystal system the relationship between lattice constants ( $a, b, c$ ) and the relationship between interaxial angles ( $\alpha, \beta, \gamma$ ). (10%)  
(b) How many Bravais crystal systems are there? (2%)
3. (a) Determine the  $c/a$  ratio of an HCP unit cell. (6 %)  
(b) Sketch the atomic arrangement of (1 1 1) plane in an FCC crystal system and give the  $[1 \bar{1} 0]$  direction on the (1 1 1) plane (5%)  
(c) The FCC and HCP structures have the same APF value of 0.74. Although both of them are close-packed structures, why are they still different? Where are the differences? (6%)
4. Consider a hypothetical metal that has a density of  $\rho = 12.0 \text{ g/cm}^3$ , an atomic weight of  $A = 131.1 \text{ g/mol}$ , and an atomic radius of  $R = 0.151 \text{ nm}$ . Compute the atomic packing factor (APF) if the unit cell is a tetragonal system, with lattice constants  $a = 0.441 \text{ nm}$  and  $c = 0.373 \text{ nm}$ . (Hint: In order to determine the APF, you have to first determine the number of atoms  $n$  in a unit cell. You will need the equation for theoretical density  $\rho = \dots$  to determine  $n$ . If you cannot solve  $n$ , then assume  $n = 3$ , you'll be able to get max. score of 5% in this case.) (12%)
5. (a) Determine the angle between plane (1 1 2) and direction  $[1 \bar{1} 1]$ . (5%) (b) Find the Miller indices of the intersection  $[u \ v \ w]$  of the planes (1 1 2) and (1 1 1). (5%) (c) Find a third plane ( $h \ k \ l$ ), on which the intersection obtained in (b) also contains. (5%)

6. X-ray diffraction result on a pure metal powder specimen reveals diffraction patterns with first five peaks at  $2\theta = 41.3^\circ, 58.2^\circ, 73.2^\circ, 87.0^\circ$ , and  $106.6^\circ$ , the wave length of X-ray emitted from a Cu target is  $\lambda = 0.1542 \text{ nm}$ .

- Index the Miller indices of the planes (h k l) of these five peaks in a correct sequence. (10%)
- For the first peak, determine the interplanar spacing  $d_{hkl}$ , the lattice constant  $a$  and atomic radius  $R$  of this metal powder. (12%)
- Check the table below to find the unknown metal powder. (4%)
- If the experiment was conducted using a powder-film X-ray diffraction, the diffraction patterns on the film are shown below. The half length of the film  $w$  is 157mm, determine the position of the second pattern  $S_2$ . (5%)



Characteristics of Selected Elements

Element	Symbol	Atomic Number	Atomic Weight (amu)	Density of Solid, 20°C (g/cm³)	Crystal Structure, 20°C	Atomic Radius (nm)	Ionic Radius (nm)	Most Common Valence	Melting Point (°C)
Aluminum	Al	13	26.98	2.71	FCC	0.143	0.053	3+	660.4
Argon	Ar	18	39.95	—	—	—	—	Inert	-189.2
Barium	Ba	56	137.33	3.5	BCC	0.217	0.136	2+	725
Beryllium	Be	4	9.012	1.85	HCP	0.114	0.035	2+	1278
Boron	B	5	10.81	2.34	Rhom.	—	0.023	3+	2300
Bromine	Br	35	79.90	—	—	—	0.196	1-	-7.2
Cadmium	Cd	48	112.41	8.65	HCP	0.149	0.095	2+	321
Calcium	Ca	20	40.08	1.55	FCC	0.197	0.100	2+	839
Carbon	C	6	12.011	2.25	Hex.	0.071	~0.016	4+	(sublimes at 3267)
Cesium	Cs	55	132.91	1.87	BCC	0.265	0.170	1+	28.4
Chlorine	Cl	17	35.45	—	—	—	0.181	1-	-101
Chromium	Cr	24	52.00	7.19	BCC	0.125	0.063	3+	1875
Cobalt	Co	27	58.93	8.9	HCP	0.125	0.072	2+	1495
Copper	Cu	29	63.55	8.94	FCC	0.128	0.096	1+	1085
Fluorine	F	9	19.00	—	—	—	0.133	1-	-220
Gallium	Ga	31	69.72	5.90	Ortho.	0.122	0.062	3+	29.8
Germanium	Ge	32	72.59	5.32	Dis. cubic	0.122	0.053	4+	937
Gold	Au	79	196.97	19.32	FCC	0.144	0.137	1+	1063
Helium	He	2	4.003	—	—	—	—	Inert	-272 (at 25 mm)
Hydrogen	H	1	1.008	—	—	—	0.154	1+	-259
Iodine	I	53	126.91	4.93	Ortho.	0.136	0.220	1-	114
Iron	Fe	26	55.85	7.87	BCC	0.124	0.077	2+	1538
Lead	Pb	82	207.2	11.35	FCC	0.175	0.120	2+	327
Lithium	Li	3	6.94	0.534	BCC	0.152	0.068	1+	181
Magnesium	Mg	12	24.31	1.74	HCP	0.160	0.072	2+	649
Manganese	Mn	25	54.94	7.44	Cubic	0.112	0.067	2+	1244
Mercury	Hg	80	200.59	—	—	—	0.110	2+	-38.8
Molybdenum	Mo	42	95.94	10.22	BCC	0.136	0.070	4+	2617
Neon	Ne	10	20.18	—	—	—	—	Inert	-248.7
Nickel	Ni	28	58.69	8.90	FCC	0.125	0.069	2+	1455
Niobium	Nb	41	92.91	8.57	BCC	0.143	0.069	5+	2468
Nitrogen	N	7	14.007	—	—	—	0.01-0.02	5+	-209.9
Oxygen	O	8	16.00	—	—	—	0.140	2-	-218.4
Phosphorus	P	15	30.97	1.82	Ortho.	0.109	0.025	5+	44.1
Platinum	Pt	78	195.08	21.45	FCC	0.139	0.080	2+	1772
Potassium	K	19	39.10	0.862	BCC	0.221	0.138	1+	63
Silicon	Si	14	28.09	2.33	Dis. cubic	0.118	0.040	4+	1410
Silver	Ag	47	107.87	10.49	FCC	0.144	0.126	1+	962
Sodium	Na	11	22.99	0.971	BCC	0.186	0.102	1+	98
Sulfur	S	16	32.06	2.07	Ortho.	0.106	0.184	2-	113
Tin	Sn	50	118.69	7.17	Tetra.	0.151	0.071	4+	232
Titanium	Ti	22	47.88	4.51	HCP	0.145	0.068	4+	1668
Tungsten	W	74	183.85	19.3	BCC	0.137	0.070	4+	3410
Vanadium	V	23	50.94	6.1	BCC	0.132	0.059	5+	1890
Zinc	Zn	30	65.39	7.13	HCP	0.133	0.074	2+	420
Zirconium	Zr	40	91.22	6.51	HCP	0.159	0.079	4+	1852

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姓名	許維驊	班別	機二A	學號	499420013

#1. (b)

$$\frac{d}{dr} E_N = \frac{d}{dr} (-Ar^{-1} + Br^{-n}) = \frac{A}{r^2} - \frac{nB}{r^{n+1}}$$

when  $r=r_0$   $\frac{d}{dr} E_N = 0$ .

$$\frac{A}{r_0^2} = \frac{nB}{r_0^{n+1}}$$

$$(r_0)^{1-n} = \frac{A}{nB} \quad r_0 = \left(\frac{A}{nB}\right)^{\frac{1}{1-n}}$$

$$E_0 = \frac{-A}{\left(\frac{A}{nB}\right)^{\frac{1}{1-n}}} + \frac{B}{\left(\frac{A}{nB}\right)^{\frac{n}{1-n}}}$$

(a)

primary: 金屬鍵, 共價鍵, 離子鍵.

secondary: 氫鍵, 凡得瓦力, 庫倫作用力.

偶極鍵.

#2.

(a)

Cubic.  $a=b=c$ .  $\alpha=\beta=\gamma=90^\circ$ .

Monoclinic  $a \neq b \neq c$   $\alpha=\beta=\gamma \neq 90^\circ$ .

Triclinic  $a \neq b \neq c$   $\alpha \neq \beta \neq \gamma \neq 90^\circ$ .

Orthorhombic  $a \neq b \neq c$   $\alpha=\beta=\gamma=90^\circ$ .

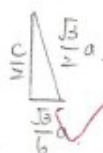
Tetragonal.  $a=b \neq c$   $\alpha=\beta=\gamma=90^\circ$ .

(b)

7. 種. 14. 種.

#3. (a).

正四面體 邊長為  $a$ , 高度  $c$ .

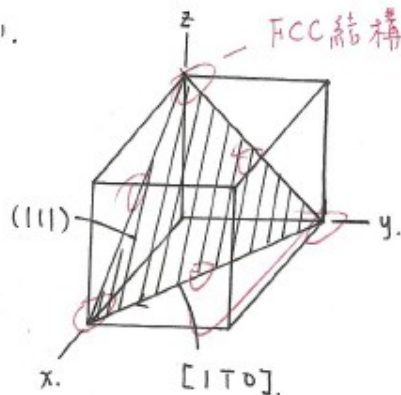


$$\frac{c}{2} = \sqrt{\frac{3}{4}a^2 - \frac{1}{4}a^2} = \sqrt{\frac{2}{3}}a$$

$$\frac{c}{a} = 2 \cdot \sqrt{\frac{2}{3}} \div 1.633$$



b1.



FCC結構原子排列需標出。

+2

(c) 原子排列順序不一樣。

HCP A B.

在(0001) ABAB排列。

FCC A B C.

在(111) ABCABC排列。

A  
B  
A  
B  
;  
A  
B  
C  
A  
B  
C  
;

+5

#4.

$\rho = 12.0 \text{ g/cm}^3$ ,  $A = 131.1 \text{ g/mol}$ , atomic  $R = 0.151 \text{ nm}$

tetragonal  $\Rightarrow a = 0.441 \text{ nm}$ ,  $c = 0.373 \text{ nm}$ .

$$APF = \frac{n \cdot \frac{4}{3} \pi (0.151)^3}{(0.441)^2 \cdot 0.373} = 0.1988n$$

+3

$$\rho = \frac{n \cdot A}{V_c \cdot N_A}$$

$$12 = \frac{n \cdot (131.1)}{\frac{4}{3} \pi (0.151 \cdot 10^{-8})^3 \cdot (6.02 \cdot 10^{23})}$$

$$12 = 15.1n, n = 0.795$$

$$\Rightarrow APF = 0.1988 \cdot 0.795 \approx 0.158$$

$$APF = \frac{n \cdot \frac{4}{3} \pi (0.151)^3}{(0.441)^2 \cdot (0.373)} = 0.79523$$

$$12 = \frac{n \cdot (131.1)}{(0.441 \cdot 10^{-8})^2 \cdot (0.373 \cdot 10^{-8}) \cdot (6.02 \cdot 10^{23})}$$

$$\Rightarrow n = 7.99 \approx 8$$

#5.

(a)  $\vec{n}_a = (1, 1, 2)$   
 $\vec{n}_b = (1, 1, 1)$

$$\vec{n}_a \cdot \vec{n}_b = |\vec{n}_a| \cdot |\vec{n}_b| \cdot \cos \theta \cdot 2.$$

$$\frac{4}{2} = 2 \cdot \sqrt{6} \cdot \sqrt{3} \cdot \cos \theta$$

$$\theta = \cos^{-1} \left( \frac{4}{2\sqrt{6} \cdot \sqrt{3}} \right) = 19.47^\circ$$

+3

(b)

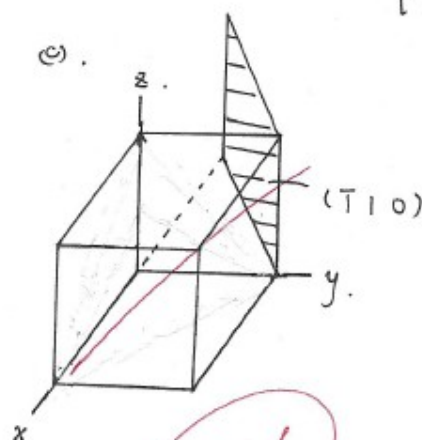
$$\vec{n}_a = (1, 1, 2)$$

$$\vec{n}_b = (1, 1, 1)$$

$$\vec{n}_a \times \vec{n}_b = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ 1 & 1 & 2 \\ 1 & 1 & 1 \end{vmatrix} = \hat{i} + 2\hat{j} + \hat{k} - \hat{k} - 2\hat{i} - \hat{j} = -\hat{i} + \hat{j}$$

$$[uvw] = [\bar{1}10].$$

+5



#6.

	$\theta$	$\sin \theta$	$\sin^2 \theta$	$(hkl)$	$N$
1.	$20.65^\circ$	0.3527	0.1244	(110)	2
2.	$29.1^\circ$	0.4863	0.2365	(200)	4
3.	$36.6^\circ$	0.5962	0.3555	(211)	6
4.	$43.5^\circ$	0.6884	0.4738	(220)	8
5.	$53.3^\circ$	0.8018	0.6428	(310)	10

+10

(a) 1<sup>st</sup> (110), 2<sup>nd</sup> (200), 3<sup>rd</sup> (211), 4<sup>th</sup> (220), 5<sup>th</sup> (310)

+12

(b) BCC,  $a = \frac{4}{\sqrt{3}} R$ ,  $n\lambda = 2 \cdot d_{hkl} \cdot \sin \theta$

$$1 \cdot 0.1542 = 2 \cdot d_{hkl} \cdot 0.3527$$

$$d_{hkl} = 0.2186 \text{ nm}$$

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$a = \sqrt{2} \cdot 0.2186$$

$$a = 0.3091 \text{ nm}$$

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

$$R = \frac{\sqrt{3}}{4} \cdot (0.3091)$$

$$R = 0.1338 \text{ nm}$$

(d)

Molybdenum.

+4

(e)

$$S_2 = 0.1542 + 0.2186 = 0.3728 \text{ nm} = 3.728 \cdot 10^{-8} \text{ mm.}$$

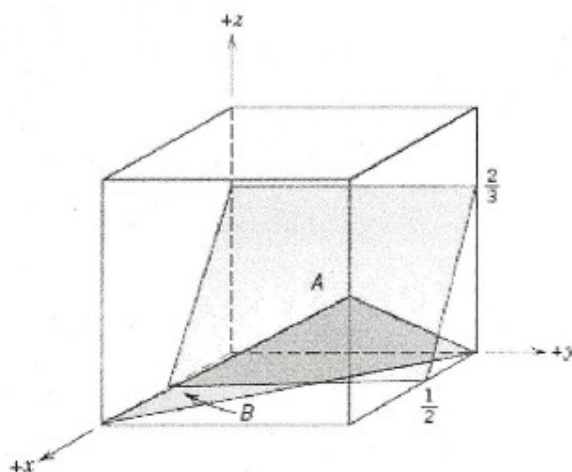
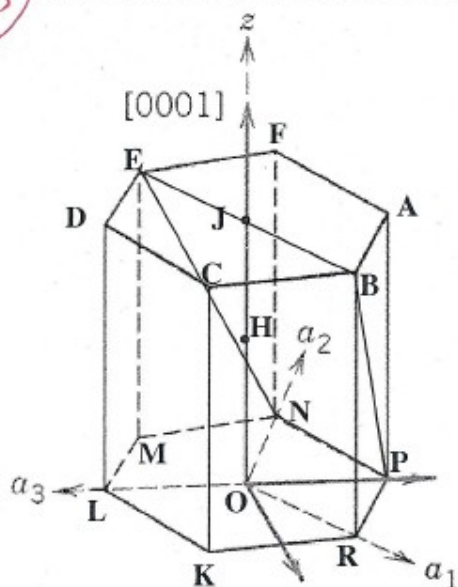
$$\frac{W}{S} = \frac{\pi}{2\theta}.$$

$$2\theta_2 = 58.2^\circ \quad \therefore S_2 = \frac{2W \cdot \theta_2}{\pi} = \frac{58.2 \cdot 157}{180} = 50.76 \text{ nm.}$$

7. Determine the Miller or Miller-Bravais indices *step by step!*

(a) Plane **EBPN** (this plane also passes through point **J** in HCP (5%))

(b) Plane **A** in cubic unit cell (5%)



(a)

$$\infty a_1 \quad 1 a_2 \quad -1 a_3 \quad 1 c.$$

$$\infty \quad 1 \quad -1 \quad 1$$

$$0 \quad 1 \quad -1 \quad 1$$

$$0 \quad 1 \quad -1 \quad 1$$

$$\left( 0 \quad 1 \quad -1 \quad 1 \right)$$

+5

(b)

$$\frac{1}{2} a \quad \infty a \quad \frac{2}{3} a.$$

$$\frac{1}{2} \quad \infty \quad \frac{2}{3}$$

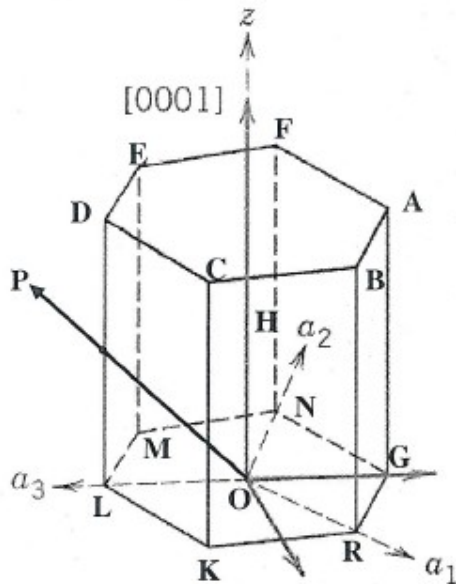
$$2 \quad 0 \quad \frac{3}{2}$$

$$4 \quad 0 \quad 3$$

$$\left( 4 \quad 0 \quad 3 \right)$$

+5

7. (c) Direction **OP** within an HCP unit cell. (5%)



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

$$\frac{1}{2} \quad \frac{1}{2} \quad 1 \quad \frac{1}{2}$$

$$-1 \quad -1 \quad 2 \quad 1$$

$$\overline{1} \quad \overline{1} \quad 2 \quad 1$$

$$[\overline{1} \quad \overline{1} \quad 2 \quad 1]$$

15