材料科学基础（双语）考试（二）试卷答案

2016~2017 学年第二学期

A 卷选择和判断答案

一、

1-10 dbaab cdacb 11-20 cbacb ddcad 21-30 cbdbd bcaad

二、

1-10 FTFFT FFTTT 11-20 FFFFF FTFFF

B 卷选择和判断答案

一、

1-10 daaab cdacb 11-20 cbabb ddcad 21-30 cbdbd bcaad

二、

1-10 FTFFT FFTTT 11-20TFFFF FTFFT

填空和大题答案

三、

1. Isotropic

2. $2\sqrt{5}R$

3.Crystalline

4.Growth

5.Cations Anions

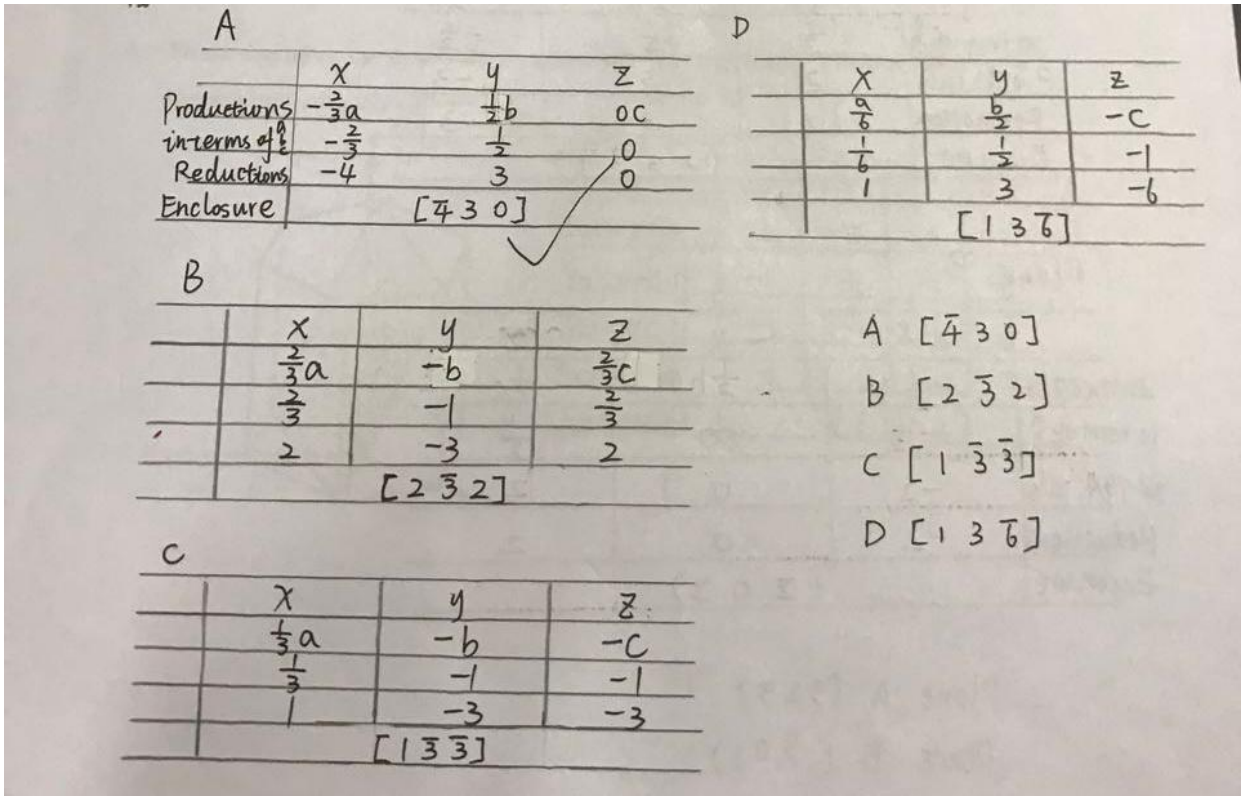
6.Graphite diamond

7.Polymorphism aolltropy

8.Smallest Translational

四、

1.


A
x y z
Productions $-\frac{2}{3}a$ $\frac{1}{2}b$ 0c
in terms of $\frac{a}{c}$ $-\frac{2}{3}$ $\frac{1}{2}$ 0
Reductions −4 3 0
Enclosure [4 3 0]
B
x y z
$\frac{2}{3}a$ −b $\frac{2}{3}c$
$\frac{2}{3}$ −1 $\frac{2}{3}$
2 −3 2
[2 $\bar{3}$ 2]
C
x y z
$\frac{1}{3}a$ −b −c
$\frac{1}{3}$ −1 −1
1 −3 −3
[1 $\bar{3}$ $\bar{3}$]
D
x y z
$\frac{a}{b}$ $\frac{b}{2}$ −c
$\frac{1}{b}$ $\frac{1}{2}$ −1
1 3 −b
[1 3 $\bar{b}$]
A [$\bar{4}$ 3 0]
B [2 $\bar{3}$ 2]
C [1 $\bar{3}$ $\bar{3}$]
D [1 3 $\bar{b}$]

2.

Plane A

	x	y	z
Intercepts	$\frac{1}{3}a$	$\frac{1}{2}b$	$-\frac{1}{2}c$
in term of $\frac{a}{b}$ $\frac{a}{c}$	$\frac{1}{3}$	$\frac{1}{2}$	$-\frac{1}{2}$
Reciprocals	3	2	-2
Reductions	3	2	-2
Enclosure		$(3\ 2\ \bar{2})$	

Plane B

	X	y	Z
Intercepts	$-\frac{1}{2}a$	∞b	$\frac{1}{2}c$
in term of $\frac{a}{b}$ $\frac{a}{c}$	$-\frac{1}{2}$	∞	$\frac{1}{2}$
Reciprocals	-2	0	2
Reductions	-2	0	2
Enclosure		$(\bar{2}\ 0\ 2)$	

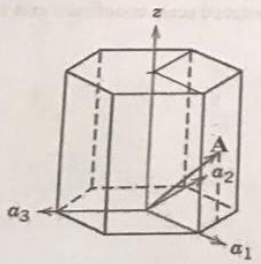
Plane A $(3\,2\,\bar{2})$

Plane B $(\bar{2}\,0\,2)$

3.

3. Please determine the indices for the directions shown in the following hexagonal unit cell.

Please show your steps. (2 points)



Solution

$[u'\ v'\ w'] = [2\ 1\ 1]$

$$\begin{cases} u = \frac{1}{3}(2u' - v') = \frac{1}{3}(4-1) = 1 \\ v = \frac{1}{3}(2v' - u') = \frac{1}{3}(2-2) = 0 \\ t = -(u+v) = -(1+0) = -1 \\ w = w' = 1 \end{cases}$$

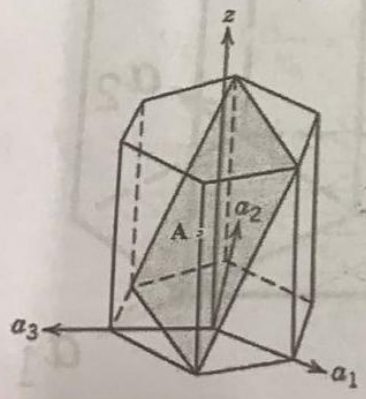
Thus, $[u\ v\ t\ w] = [1\ 0\ \bar{1}\ 1]$

The indices for the direction A is $[1\,0\,\bar{1}\,1]$.

4.

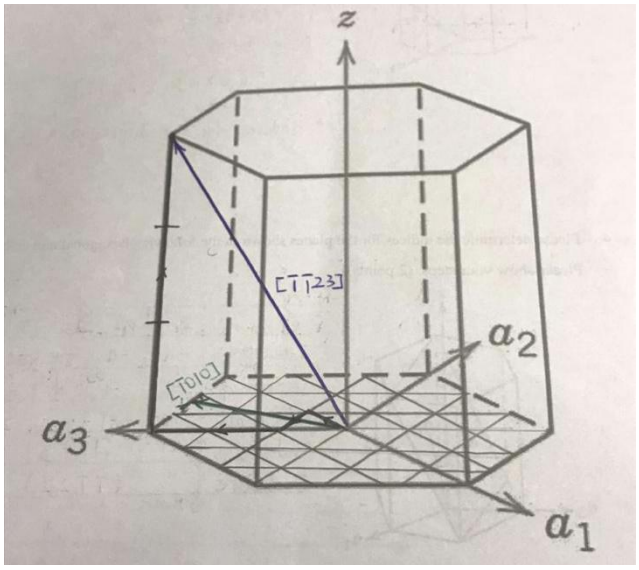
4. Please determine the indices for the planes shown in the following hexagonal unit cell.

Please show your steps. (2 points)



	a_1	a_2	a_3	z
Intercepts	-a	-a	$\frac{1}{2}$a	$\frac{1}{2}$c
in terms of	-1	-1	$\frac{1}{2}$	$\frac{1}{2}$
Reciprocals	-1	-1	2	2
Reductions	-1	-1	2	2
Enclosure	($\bar{1}\bar{1}$22)			

5.

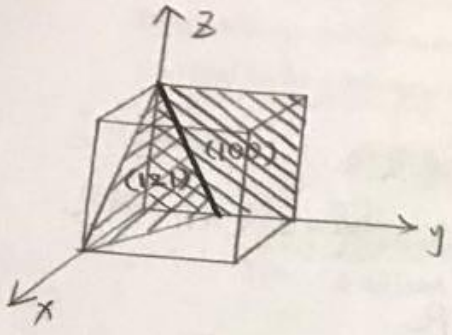


五、

1.

V. Please solve the following problems with detailed steps. (43 points)

1. 求由晶面(121)与(100)所决定的晶带轴指数. (5 Points)



晶带轴指数为 [01$\bar{2}$]

2.

2. Titanium has an HCP crystal structure and a density of 4.51 g/cm³.

(1) What is the volume of its unit cell in cubic meters?

(2) If the *c*/*a* ratio is 1.58, compute the values of *c* and *a*. (6 points)

Ti : Atomic weight: 47.87g/mol

Solution

(1) According to the density equation

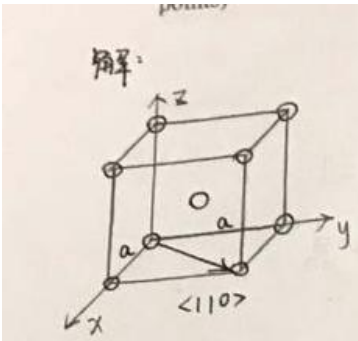
$$V_C = \frac{nA}{\rho \cdot N_A} = \frac{(6\ \text{atoms/unit cell}) \times (47.87\ \text{g/mol})}{(4.51\ \text{g/cm}^3) \times (6.023 \times 10^{23}\ \text{atom/mol})} = 1.057 \times 10^{-22}\ \text{cm}^3/\text{unit cell}$$

(2) $V = 3V_{para} = 3 \times (a \times \frac{\sqrt{3}}{2} a \times c) = \frac{3\sqrt{3}}{2} \times 1.58 \times a^3 = 1.057 \times 10^{-22}\ \text{cm}^3$

Thus, $a = \sqrt[3]{0.3575 \times 10^{-22}\ \text{cm}^3} = 0.295 \times 10^{-7}\ \text{cm} = 0.295\ \text{nm}$

$C = 1.58a = 0.466\ \text{nm}$

3.



沿 <110> 晶向有:

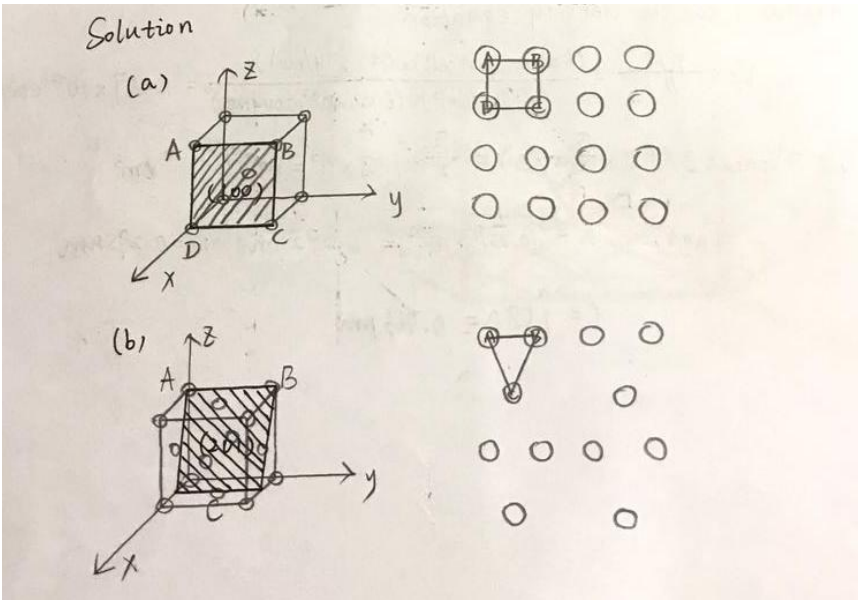
$\sqrt{2}a = 2R + d$

d为八面体间隙直径.

$\Rightarrow d = \sqrt{2}a - 2R = (\frac{4\sqrt{2}}{\sqrt{3}} - 2)R = 1.266R$

$\therefore r = \frac{d}{2} = 0.633R$.

4.



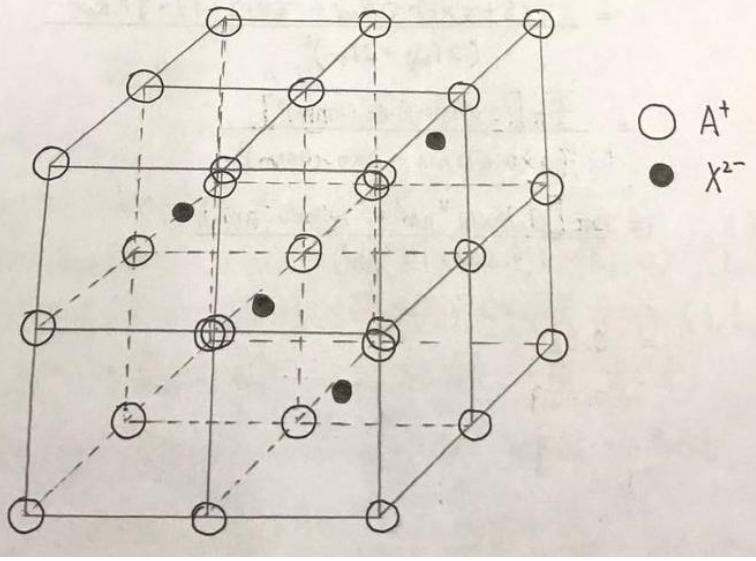
5.

Solution

(a) $\frac{r_{A^+}}{r_{X^{2-}}} = \frac{0.125nm}{0.145nm} = 0.862 \in (0.732, 1)$

Thurs, the coordination number for each A^+ is 8.

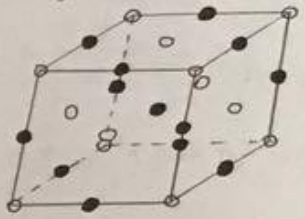
(b). The crystal structure for AX should be similiar to Fluorite.



6.

Solution

MgO has the same crystal struction of NaCl.



Ionic radius of Mg^{2+}: 0.072nm

O^{2-}: 0.140nm

$$IPF = \frac{n_{Mg^{2+}} \times V_{Mg^{2+}} + n_{O^{2-}} \times V_{O^{2-}}}{a^3}$$

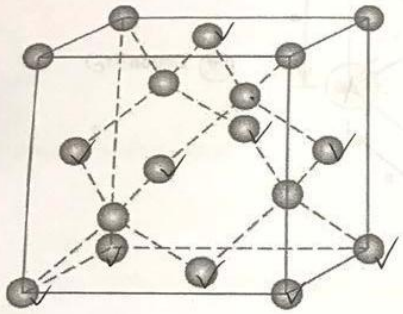
$$= \frac{(\frac{1}{8}\times 8 + \frac{1}{2}\times 6)\times \frac{4}{3}\pi R_{Mg^{2+}}^3 + (\frac{1}{4}\times 12 + 1)\times \frac{4}{3}\pi R_{O^{2-}}^3}{(2r_{Mg^{2+}} + 2r_{O^{2-}})^3}$$

$$= \frac{\frac{16}{3}\pi[(0.072nm)^3 + (0.140nm)^3]}{(2\times 0.072nm + 2\times 0.140nm)^3}$$

$$= \frac{2\pi[3.73\times 10^{-4}nm^3 + 2.744\times 10^{-3}nm^3]}{3\times (9.528\times 10^{-3}nm^3)}$$

$$= 0.69$$

7.



Si

$\frac{\sqrt{3}}{4}a = 2R$.

Atomic radii of Si: 0.118 nm

Solution

The crystal structure of Si is similar to ZnS.

The coordinations of Si: (0,0,0). (0,0,1). (0,1,0). (1,1,0), (1,0,1). (1,0,0). (0,1,1). (1,1,1).

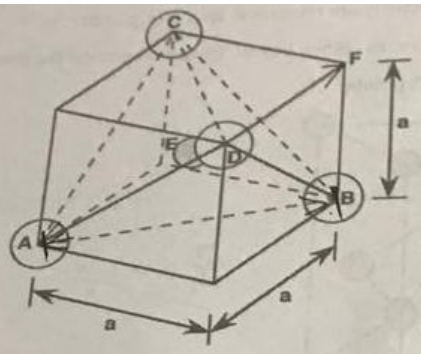
$(\frac{1}{2},0,\frac{1}{2})$. $(\frac{1}{2},\frac{1}{2},0)$. $(0,\frac{1}{2},\frac{1}{2})$. $(\frac{1}{2},1,\frac{1}{2})$. $(\frac{1}{2},\frac{1}{2},1)$. $(1,\frac{1}{2},\frac{1}{2})$..

$(\frac{1}{4},\frac{1}{4},\frac{3}{4})$. $(\frac{1}{4},\frac{3}{4},\frac{1}{4})$. $(\frac{3}{4},\frac{1}{4},\frac{1}{4})$. $(\frac{3}{4},\frac{3}{4},\frac{3}{4})$.

Thus, along the [111], there are two atoms in total.

$$LD_{[111]} = \frac{2\text{ atoms}}{\sqrt{3}a} = \frac{2\text{ atoms}}{\sqrt{3}\times\frac{2R}{\frac{\sqrt{3}}{4}}} = \frac{1}{4R} = \frac{1}{4\times 0.118\text{nm}} = 2.119\ \text{nm}^{-1}$$

8.



Solution

① $AB = 2r_A = \sqrt{2}\,a$

$\Rightarrow a = \sqrt{2}\,r_A$ ← There will be an anion located at F position.

② $AEF = 2r_A + 2r_C = \sqrt{AB^2 + BF^2}$

$= \sqrt{4r_A^2 + 2r_A^2} = \sqrt{6}\,r_A$

$\Rightarrow 2 + 2\frac{r_C}{r_a} = \sqrt{6}$

Thus, $\frac{r_C}{r_a} = \frac{\sqrt{6}-2}{2} = 0.225$