苏泓源 2019010448 固物 HW3

1、

简单立方

$$\begin{cases}\vec{\alpha}_1 = a\vec{i}\\ \vec{\alpha}_2 = a\vec{j}\\ \vec{\alpha}_3 = a\vec{k}\end{cases} \quad 另一组 \quad \begin{cases}\vec{\alpha}_1' = -a\vec{i}\\ \vec{\alpha}_2 = a\vec{j}\\ \vec{\alpha}_3 = a\vec{k}\end{cases}$$

体心立方

$$\begin{cases}\vec{\alpha}_1 = \frac{a}{2}(-\vec{i}+\vec{j}+\vec{k})\\ \vec{\alpha}_2 = \frac{a}{2}(\vec{i}-\vec{j}+\vec{k})\\ \vec{\alpha}_3 = \frac{a}{2}(\vec{i}+\vec{j}-\vec{k})\end{cases} \quad 另一组 \quad \begin{cases}\vec{\alpha}_1 = \frac{a}{2}(-\vec{i}-\vec{j}-\vec{k})\\ \vec{\alpha}_2 = \frac{a}{2}(\vec{i}-\vec{j}+\vec{k})\\ \vec{\alpha}_3 = \frac{a}{2}(\vec{i}+\vec{j}-\vec{k})\end{cases}$$

面心立方

$$\begin{cases}\vec{\alpha}_1 = \frac{a}{2}(\vec{j}+\vec{k})\\ \vec{\alpha}_2 = \frac{a}{2}(\vec{i}+\vec{k})\\ \vec{\alpha}_3 = \frac{a}{2}(\vec{i}+\vec{j})\end{cases} \quad 另一组 \quad \begin{cases}\vec{\alpha}_1 = \frac{a}{2}(\vec{i}-\vec{k})\\ \vec{\alpha}_2 = \frac{a}{2}(\vec{i}+\vec{k})\\ \vec{\alpha}_3 = \frac{a}{2}(\vec{i}+\vec{j})\end{cases}$$

两组基矢比较：

① 每个基矢长度相同

② 基矢围成的平行六面体体积相同.

③ $\vec{\alpha}_2'$ 与 $\vec{\alpha}_2$，$\vec{\alpha}_3'$ 与 $\vec{\alpha}_3$ 相同，$\vec{\alpha}_1$、$\vec{\alpha}_1'$ 关于 $\vec{\alpha}_2\times\vec{\alpha}_3$ 对称.

2. $\vec{a}=3\vec{i}$，$\vec{b}=3\vec{j}$，$\vec{c}=\frac{3}{2}(\vec{i}+\vec{j}+\vec{k})$

原胞体积 $V_1=|\vec{\alpha}_1\cdot(\vec{\alpha}_2\times\vec{\alpha}_3)| = 13.5\,nm^3$

单胞体积 $V_2=|a|^3 = 27\,nm^3$

属于体心立方

3.

1) $\frac{\sqrt{3}}{4}a = 2.45\,Å$

2) $\frac{\sqrt{2}}{2}a = 4.00\,Å$

4.

简单立方，1个格点，$r_{max} = \frac{a}{2}$

$K_1 = 1\cdot\frac{4}{3}\pi r_{max}^3/a^3 = \frac{\pi}{6}$

面心立方：4个格点，$r_{max} = \frac{\sqrt{2}}{4}a$

$K_2 = 4\cdot\frac{4}{3}\pi r_{max}^3/a^3 = 4\cdot\frac{4}{3}\pi\cdot\left(\frac{\sqrt{2}}{4}\right)^3 = \frac{\sqrt{2}}{6}\pi$

体心立方：2个格点，$r_{max} = \frac{\sqrt{3}}{4}a$

$K_3 = 2\cdot\frac{4}{3}\pi r_{max}^3/a^3 = 2\cdot\frac{4}{3}\pi\cdot\left(\frac{\sqrt{3}}{4}\right)^3 = \frac{\sqrt{3}}{8}\pi$

六角密排：6个格点，$r_{max} = \frac{1}{2}a$

$K_4 = 6\cdot\frac{4}{3}\pi r_{max}^3 \Big/ \frac{3\sqrt{3}}{2}a^2\cdot\frac{\sqrt{8}}{\sqrt{3}}a = \frac{\sqrt{2}}{6}\pi$

5.

简单立方：{100}

体心立方：{110}

面心立方：{111}

6. 对于{110}，考虑到体心到角中点，存在格点，

$d_{\{110\}} = \frac{\sqrt{2}}{2}a/2 = \frac{\sqrt{2}}{4}a = 1.92\,Å$

对于{111}，可等效为面心立方沿对角线平移 $\frac{\sqrt{3}}{4}a$，同理根据正四面体性质，还有 $d = \frac{\sqrt{3}}{12}a$

∴ 有2种间距

$$d_{\{111\}} = \begin{cases}\frac{\sqrt{3}}{4}a\\ \frac{\sqrt{3}}{12}a\end{cases}$$

7.

1)

ED: $\langle 1\bar{1}1 \rangle$ FD: $\langle 1\bar{1}0 \rangle$

OF: $\langle 011 \rangle$

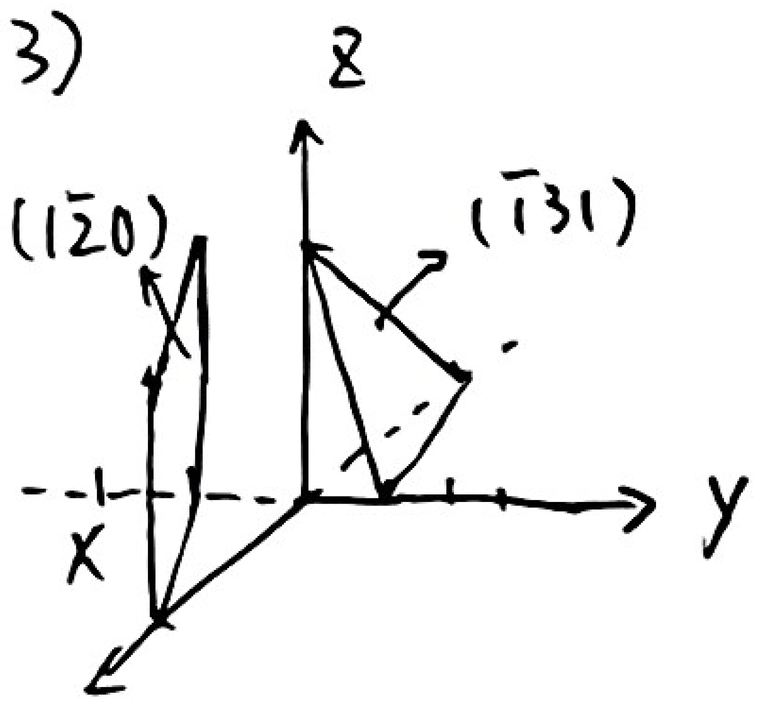
2)

FGIH: (201)

AGK: $(1\bar{1}1)$

MNLK: $(2\bar{1}0)$

3)



4) $d = \left[(1,1,1)\cdot(1,0,0) \big/ |(1,1,1)| \right] a$

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

8.

以O为原点建立abc直角坐标系

$\vec{OA} = (1,1,0)$ $\vec{OB} = (0, \frac{1}{2}, \frac{1}{2})$

$\vec{OC} = (\frac{1}{2}, \frac{1}{2}, 1)$

$\therefore \vec{AB} = \vec{OB} - \vec{AO} = (-1, -\frac{1}{2}, \frac{1}{2})$

$\vec{AC} = \vec{OC} - \vec{AO} = (-\frac{1}{2}, -\frac{1}{2}, 1)$

$\therefore$ 面ABC法向量 $\vec{n} = (1,-3,-1)$

$\therefore$ 密勒指数为 $(1\bar{3}\bar{1})$ 或 $(\bar{1}31)$

思考题

1、

指数低，因为晶面指数低意味着晶面间距更大，原子间键数少，更容易沿该晶面分裂。

2.

面心立方格子：8个顶点和6个面心

简单立方格子：