苏泓源 2019010448 固物 HW4

1、

$\lambda = h/p, \quad \frac{p^2}{2m_e} = eV$

$\therefore \lambda = \frac{h}{\sqrt{2m_e eV}} \approx 0.388\,\text{Å}$

对(100)面, $d = a = 1\,\text{Å}$

第一级衍射极大布拉格角$\theta$满足

$2d\sin\theta = \lambda$

$\therefore \theta = \arcsin\frac{\lambda}{2d} = 11.18°$

2.

证明

对面心立方

$$\begin{cases} \vec{\alpha}_1 = \frac{a}{2}(\vec{j}+\vec{k}) \\ \vec{\alpha}_2 = \frac{a}{2}(\vec{k}+\vec{i}) \\ \vec{\alpha}_3 = \frac{a}{2}(\vec{i}+\vec{j}) \end{cases} \qquad \begin{cases} \vec{b}_1 = \frac{2\pi}{a}(-\vec{i}+\vec{j}+\vec{k}) \\ \vec{b}_2 = \frac{2\pi}{a}(\vec{i}-\vec{j}+\vec{k}) \\ \vec{b}_3 = \frac{2\pi}{a}(\vec{i}+\vec{j}-\vec{k}) \end{cases}$$

对体心立方

$\vec{\alpha}_1' = \frac{a}{2}(-\vec{i}+\vec{j}+\vec{k})$ 与 $\vec{b}_1$ 方向相同

$\vec{\alpha}_2' = \frac{a}{2}(\vec{i}-\vec{j}+\vec{k})$ 与 $\vec{b}_2$ 方向相同

$\vec{\alpha}_3' = \frac{a}{2}(\vec{i}+\vec{j}-\vec{k})$ 与 $\vec{b}_3$ 方向相同

$\vec{b}_1' = \frac{2\pi}{a}(\vec{j}+\vec{k})$ 与 $\vec{\alpha}_1$ 方向相同

$\vec{b}_2' = \frac{2\pi}{a}(\vec{k}+\vec{i})$ 与 $\vec{\alpha}_2$ 方向相同

$\vec{b}_3' = \frac{2\pi}{a}(\vec{i}+\vec{j})$ 与 $\vec{\alpha}_3$ 方向相同

∴ 晶格互为倒易点阵

面心立方晶格第一布里渊区为14面体，由原点和最邻近8个倒格点连线的垂直平分面围成的8面体，与6个次邻近倒格点连线的垂直平分面割去6个角形成

3、

G格子原胞体积

$V_c = \vec{\alpha}_1\cdot(\vec{\alpha}_2\times\vec{\alpha}_3) = \vec{\alpha}_2\cdot(\vec{\alpha}_3\times\vec{\alpha}_1) = \vec{\alpha}_3\cdot(\vec{\alpha}_1\times\vec{\alpha}_2)$

倒格子原胞体积

$V_b = \vec{b}_1\cdot(\vec{b}_2\times\vec{b}_3)$

$= \frac{2\pi(\vec{\alpha}_2\times\vec{\alpha}_3)}{\vec{\alpha}_1\cdot(\vec{\alpha}_2\times\vec{\alpha}_3)}\cdot\left(\frac{2\pi(\vec{\alpha}_3\times\vec{\alpha}_1)}{\vec{\alpha}_2\cdot(\vec{\alpha}_3\times\vec{\alpha}_1)}\times\frac{2\pi(\vec{\alpha}_1\times\vec{\alpha}_2)}{\vec{\alpha}_3\cdot(\vec{\alpha}_1\times\vec{\alpha}_2)}\right)$

$= \frac{(2\pi)^3}{V_c^3}\cdot(\vec{\alpha}_2\times\vec{\alpha}_3)\cdot\left[(\vec{\alpha}_3\times\vec{\alpha}_1)\times(\vec{\alpha}_1\times\vec{\alpha}_2)\right]$

由 $A\times(B\times C) = (A\cdot C)B - (A\cdot B)C$

$\therefore (\vec{\alpha}_3\times\vec{\alpha}_1)\times(\vec{\alpha}_1\times\vec{\alpha}_2)$

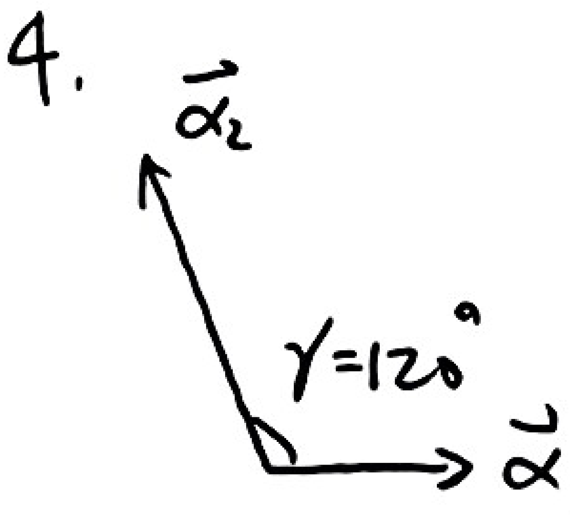
$= \left[(\vec{\alpha}_3\times\vec{\alpha}_1)\cdot\vec{\alpha}_2\right]\vec{\alpha}_1 - \left[\overbrace{(\vec{\alpha}_3\times\vec{\alpha}_1)\cdot\vec{\alpha}_1}^{0}\right]\vec{\alpha}_2$

$= \left[(\vec{\alpha}_3\times\vec{\alpha}_1)\cdot\vec{\alpha}_2\right]\vec{\alpha}_1 = V_c\vec{\alpha}_1$

$\therefore V_b = \frac{(2\pi)^3}{V_c^3}\cdot(\vec{\alpha}_2\times\vec{\alpha}_3)\cdot V_c\vec{\alpha}_1$

$= (2\pi)^3/V_c$

4.



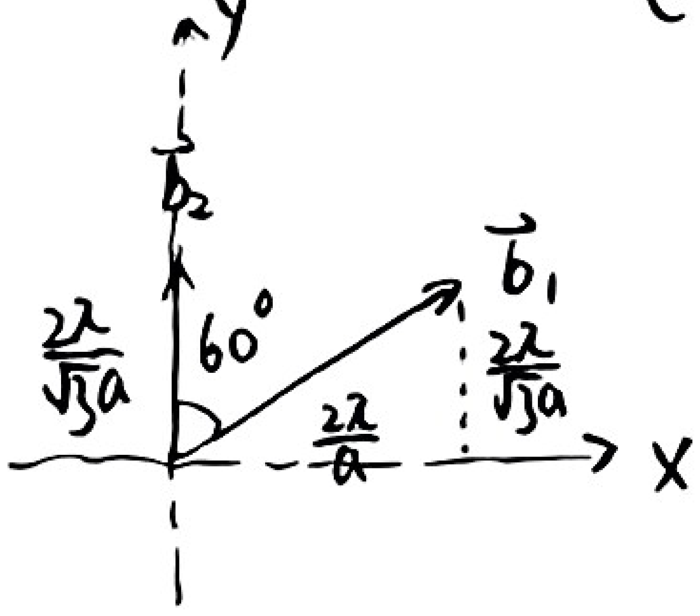

$\vec{\alpha}_1 = (a, 0)$

$\vec{\alpha}_2 = (-a, \sqrt{3}a)$

$a = 1.25\,\text{Å}$

$\therefore \vec{b}_1 = 2\pi\cdot\frac{\begin{bmatrix}0&1\\-1&0\end{bmatrix}\begin{pmatrix}-a\\\sqrt{3}a\end{pmatrix}}{(a,0)\begin{bmatrix}0&1\\-1&0\end{bmatrix}\begin{pmatrix}-a\\\sqrt{3}a\end{pmatrix}} = \frac{2\pi}{a}\begin{pmatrix}1\\1/\sqrt{3}\end{pmatrix}$

$\vec{b}_2 = 2\pi\cdot\frac{\begin{bmatrix}0&1\\-1&0\end{bmatrix}\begin{pmatrix}a\\0\end{pmatrix}}{(-a,\sqrt{3}a)\begin{bmatrix}0&1\\-1&0\end{bmatrix}\begin{pmatrix}a\\0\end{pmatrix}} = \frac{2\pi}{a}\begin{pmatrix}0\\1/\sqrt{3}\end{pmatrix}$



5.

证明

$$\begin{cases}\vec{a_1}=a\vec{i}\\ \vec{a_2}=b\vec{j}\\ \vec{a_3}=c\vec{k}\end{cases} \Rightarrow \begin{array}{l}\vec{b_1}=\frac{2\pi}{a}\vec{i}\\ \vec{b_2}=\frac{2\pi}{b}\vec{j}\\ \vec{b_3}=\frac{2\pi}{c}\vec{k}\end{array}$$

$$\therefore \vec{G}=h\vec{b_1}+k\vec{b_2}+l\vec{b_3}=2\pi\left(\frac{h}{a}\vec{i}+\frac{k}{b}\vec{j}+\frac{l}{c}\vec{k}\right)$$

$$\therefore d_{hkl}=\frac{2\pi}{|\vec{G}|}=1\Big/\sqrt{\left(\frac{h}{a}\right)^2+\left(\frac{k}{b}\right)^2+\left(\frac{l}{c}\right)^2}$$

6.

每个波矢态体积

$$\Delta k_x\Delta k_y\Delta k_z=\frac{(2\pi)^3}{N_1N_2N_3\cdot a^3}$$

对面心立方晶格，$V_c=\frac{1}{4}a^3$

倒格子体积 $V_b=(2\pi)^3/V_c=\frac{8\pi^3}{V_c}=\frac{32\pi^3}{a^3}$

∴波矢状态数为

$$n=V_b/\Delta k_x\Delta k_y\Delta k_z=\frac{32\pi^3/a^3}{(2\pi)^3/a^3\cdot N_1\cdot N_2\cdot N_3}$$

$$=4N_1N_2N_3$$

7.

a) $2d\sin\theta=\lambda \Rightarrow d=\frac{\lambda}{2\sin\theta}=\frac{\lambda}{2\sin\frac{\varphi}{2}}=2.17\text{Å}$

b) $8g/cm^3=8\times10^6 g/m^3$

$$n=\frac{8\times10^6}{64}\times N_0=7.525\times10^{28}$$

c)

若简单立方，惯用晶胞边长为 $\overset{a_1=}{\vee}\ {}^{1/3}\!\sqrt{n}=2.37\text{Å}$

晶面间距最大为 $a_1=2.37\text{Å}\neq2.17\text{Å}$，不符合

若面心立方，$a_2={}^{1/3}\!\sqrt{n/4}\approx3.76\text{Å}$

最大晶面间距 $d=\frac{\sqrt{3}}{3}a_2=2.17\text{Å}=2.17\text{Å}$

符合要求

若体心立方，$a_3={}^{1/3}\!\sqrt{n/2}=2.98\text{Å}$

最大晶面间距 $d=\frac{\sqrt{2}}{2}a_3=2.11\text{Å}\neq2.17\text{Å}$

不符合要求

综上所述，金属晶体为面心立方。