北京大学 PEKING UNIVERSITY

HW 4

1.12:

晶格	晶系	Bravais格子	点群	空间群
面心立方晶格	立方	面心立方	O_h	$(\hat{R}\|\vec{t}_{l_1l_2l_3})$, $\hat{R}\in O_h$
金刚石晶格	立方	面心立方	T_d	$(\hat{R}\|\vec{t}_{l_1l_2l_3}+\vec{\tau})$ $\begin{cases}\hat{R}\notin T_d,\ \hat{R}\in O_h.\ \vec{\tau}=\frac{a}{4}(\vec{i}+\vec{j}+\vec{k})\\ \hat{R}\in T_d.\ \vec{\tau}=\vec{0}\end{cases}$
闪锌矿晶格	立方	面心立方	T_d	$(\hat{R}\|\vec{t}_{l_1l_2l_3})$, $\hat{R}\in T_d$
NaCl晶格	立方	简立方	O_h	$(\hat{R}\|\vec{t}_{l_1l_2l_3})$, $\hat{R}\in O_h$

平移群 $\vec{R}_{l_1l_2l_3}=l_1\vec{a}_1+l_2\vec{a}_2+l_3\vec{a}_3$

2.a. 二维倒格 $\vec{b}_1=\frac{2\pi\,\vec{a}_2\times\vec{a}_3}{S}$ $\vec{b}_2=\frac{2\pi}{S}(\vec{a}_3\times\vec{a}_1)$

$\therefore S^*=\vec{b}_1\cdot(\vec{b}_2\times\vec{a}_3)\,|\vec{b}_1\times\vec{b}_2|$ $(A\times B)\times C=(A\cdot C)B-(A\cdot B)C$

$=(\frac{2\pi}{S})^2\cdot|(\vec{a}_2\times\vec{a}_3)\times(\vec{a}_3\times\vec{a}_1)|$

$=(\frac{2\pi}{S})^2|(\vec{a}_1\times\vec{a}_3)\times(\vec{a}_2\times\vec{a}_3)|=(2\pi)^2/S$

2. S_1: $\hat{E}$. $\hat{\sigma}$ $\{\hat{E},\hat{\sigma}\}$

S_2: $\hat{S}_2=\hat{C}_2^1\times\hat{\sigma}=\hat{i}$ $(\hat{S}_2)^2=\hat{E}$ $\{\hat{E},\hat{i}\}$

S_3: $\hat{S}_3=\hat{\sigma}\times\hat{C}_3^1$ $(\hat{S}_3)^2=\hat{C}_3^2$.

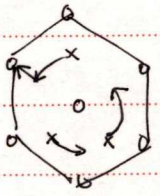
$(\hat{S}_3^3)=\hat{\sigma}$ $(\hat{C}_3^4)=\hat{C}_3^1$ $(\hat{S}_3^5)=\hat{\sigma}\hat{C}_3^2$ $(\hat{S}_3^6)=\hat{E}$

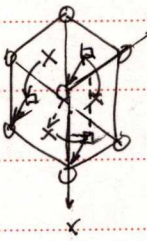
S_4: $\hat{S}_4=\hat{\sigma}\hat{C}_4^1$ $\hat{S}_4^2=\hat{C}_2^1$ $\hat{S}_4^3=\hat{\sigma}\hat{C}_4^3$ $\hat{S}_4^4=\hat{i}$

S_6: $\hat{S}_6=\sigma C_6^1$ $S_6^2=\sigma C_3$ $S_6^3=\sigma C_2^1=i$

$S_6^4=C_3^2$ $S_6^5=\sigma C_6^5$ $S_6^6=E$.

4.





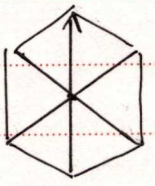
沿中心轴进行 D_{6h} 但不同于 D_{3h} 中的

如 $\hat{C}_6$，x位原子 → 口位，o位仍o位

施行 $\frac{a}{3}\vec{e}_x - \frac{a}{3}\vec{e}_y + \frac{a}{2}\vec{e}_z$，□→○，○→□.

记单，$\therefore \vec{T} \neq 0$，记单.

5.



$\theta = n\frac{\pi}{3}$ $(n \in \mathbb{Z})$：D_{6h}

$\theta = n\frac{\pi}{3} + \frac{\pi}{6}$ D_{6d}

没有这样的 D_6.