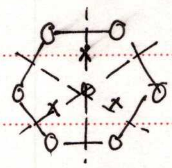
HW 3

1. Pf: A 操作矩阵为 $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}$ C 操作矩阵为 $\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$

B 操作矩阵为 $\cancel{\begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}}$ $\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

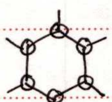
$\therefore BA = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} = C.$ 证毕.

2. 六角密排单胞对称操作: C_3^1. C_3^2. E. $3C_2^1$. $3m$. σ_h. S_3^1. S_3^2.

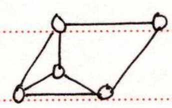


D_{3h} 群 12阶.

3. 石墨烯: (存疑)



原胞



二维: 10种点群

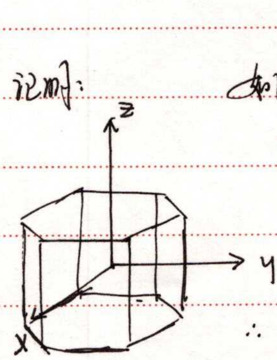
C_1. C_2 C_3. C_4. C_6

C_v. C_{2v}. C_{3v}. C_{4v}. C_{6v}

2D石墨烯单胞为六角形. 原胞为平行四边形.

∴ 石墨烯最大点群 = 二维的最大点群 = C_{6v}. "对称面 → 对称线"

4. 证明: (a) ~~如图~~将电场与晶体沿z旋转 $\pi/3$.



(a)

则矩阵为 $A = \begin{pmatrix} \frac{\sqrt{3}}{2} & -\frac{1}{2} & \\ \frac{1}{2} & \frac{\sqrt{3}}{2} & \\ & & 1 \end{pmatrix}$

$$\begin{cases} \cancel{\varepsilon_{xx} = \frac{\sqrt{3}}{2}\varepsilon_{xx} - \frac{1}{2}\varepsilon_{yx}} \\ \cancel{\varepsilon_{xy} = \frac{\sqrt{3}}{2}\varepsilon_{xy} - \frac{1}{2}\varepsilon_{yy}} \\ \cancel{\varepsilon_{yx} = \frac{1}{2}\varepsilon_{xx} + \frac{\sqrt{3}}{2}\varepsilon_{yx}} \\ \cancel{\varepsilon_{yy} = \frac{1}{2}\varepsilon_{xy} + \frac{\sqrt{3}}{2}\varepsilon_{yy}} \end{cases}$$

$\therefore \varepsilon = A^T \varepsilon A$

$$= \begin{pmatrix} \frac{\sqrt{3}}{2}\varepsilon_{11} + \frac{1}{2}\varepsilon_{21}, & \frac{\sqrt{3}}{2}\varepsilon_{12} + \frac{1}{2}\varepsilon_{22}, & \frac{\sqrt{3}}{2}\varepsilon_{13} + \frac{1}{2}\varepsilon_{23} \\ -\frac{1}{2}\varepsilon_{11} + \frac{\sqrt{3}}{2}\varepsilon_{21}, & -\frac{1}{2}\varepsilon_{12} + \frac{\sqrt{3}}{2}\varepsilon_{22}, & -\frac{\sqrt{3}}{2}\varepsilon_{13} + \frac{\sqrt{3}}{2}\varepsilon_{23} \\ \varepsilon_{13} & \varepsilon_{23} & \varepsilon_{33} \end{pmatrix} \begin{pmatrix} \frac{\sqrt{3}}{2} & -\frac{1}{2} & \\ \frac{1}{2} & \frac{\sqrt{3}}{2} & \\ & & 1 \end{pmatrix}$$

$$
=\begin{pmatrix}
\frac{3}{4}\varepsilon_{11}+\frac{\sqrt{3}}{4}\varepsilon_{21}+\frac{\sqrt{3}}{4}\varepsilon_{12}+\frac{1}{4}\varepsilon_{22}, & -\frac{\sqrt{3}}{4}\varepsilon_{11}-\frac{1}{4}\varepsilon_{21}+\frac{3}{4}\varepsilon_{12}+\frac{\sqrt{3}}{4}\varepsilon_{22}, & \frac{\sqrt{3}}{2}\varepsilon_{13}+\frac{1}{2}\varepsilon_{23} \\
-\frac{\sqrt{3}}{4}\varepsilon_{11}+\frac{3}{4}\varepsilon_{21}-\frac{1}{4}\varepsilon_{12}+\frac{\sqrt{3}}{4}\varepsilon_{22}, & \frac{1}{4}\varepsilon_{11}-\frac{\sqrt{3}}{4}\varepsilon_{21}-\frac{\sqrt{3}}{4}\varepsilon_{12}+\frac{3}{4}\varepsilon_{22}, & -\frac{1}{2}\varepsilon_{13}+\frac{\sqrt{3}}{2}\varepsilon_{23} \\
\frac{\sqrt{3}}{2}\varepsilon_{13}+\frac{1}{2}\varepsilon_{23}, & -\frac{1}{2}\varepsilon_{13}+\frac{\sqrt{3}}{2}\varepsilon_{23}, & \varepsilon_{33}
\end{pmatrix}
$$

$\therefore\ \varepsilon_{13}=\varepsilon_{23}=0.$

$$
\begin{cases}
\varepsilon_{11}=\frac{3}{4}\varepsilon_{11}+\frac{\sqrt{3}}{4}\varepsilon_{21}+\frac{\sqrt{3}}{4}\varepsilon_{12}+\frac{1}{4}\varepsilon_{22} & ① \\
\varepsilon_{22}=\frac{1}{4}\varepsilon_{11}-\frac{\sqrt{3}}{4}\varepsilon_{21}-\frac{\sqrt{3}}{4}\varepsilon_{12}+\frac{3}{4}\varepsilon_{22} & ② \\
\varepsilon_{12}=-\frac{\sqrt{3}}{4}\varepsilon_{11}-\frac{1}{4}\varepsilon_{21}+\frac{3}{4}\varepsilon_{12}+\frac{\sqrt{3}}{4}\varepsilon_{22} & ③ \\
\varepsilon_{21}=-\frac{\sqrt{3}}{4}\varepsilon_{11}+\frac{3}{4}\varepsilon_{21}-\frac{1}{4}\varepsilon_{12}+\frac{\sqrt{3}}{4}\varepsilon_{22} & ④
\end{cases}
$$

$\cancel{③-④\quad \varepsilon_{12}-\varepsilon_{21}=\varepsilon_{12}-}$

$③+④\quad \varepsilon_{12}+\varepsilon_{21}=-\frac{\sqrt{3}}{2}(\varepsilon_{11}-\varepsilon_{22})+\frac{1}{2}(\varepsilon_{12}+\varepsilon_{21})$

$①-②\quad \varepsilon_{11}-\varepsilon_{22}=\frac{1}{2}(\varepsilon_{11}-\varepsilon_{22})+\frac{\sqrt{3}}{2}(\varepsilon_{21}+\varepsilon_{12})$

$\therefore\ \varepsilon_{12}+\varepsilon_{21}=\varepsilon_{11}-\varepsilon_{22}=0$

又 $\because\ \varepsilon_{12}=\varepsilon_{21}\quad \therefore\ \varepsilon_{12}=\varepsilon_{21}=0$

由于存在σ_v. 对σ_v的操作 $x\to x.\ y\to -y.\ z\to z$

$\therefore\ \varepsilon_{xy}=-\varepsilon_{xy}=0.\quad (\varepsilon_{12}=-\varepsilon_{12}=0)\Rightarrow\ \varepsilon_{21}=\varepsilon_{12}=0$ 证毕.