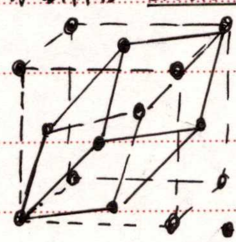
HW2

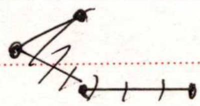
1. 立方金刚石 Bravais格子原胞

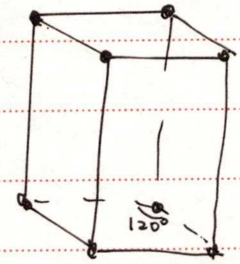


● 阵点,

每一个阵点代表一个正格矢 $\vec{R_l}$

六方金刚石 Bravais 原胞:



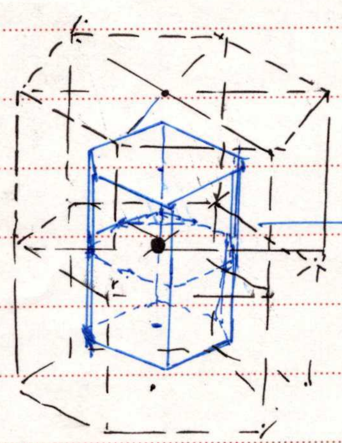


●: 阵点.

Bravais 格子: 正格矢 $\vec{R_l} = l_1\vec{a_1} + l_2\vec{a_2} + l_3\vec{a_3}$ 表示空间中的点

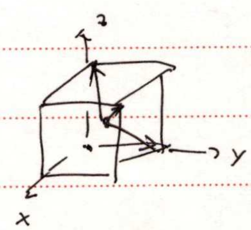
组成了阵点, 格子.

区别: 其中一个是正格矢, 另外一个是原子(阵点位于原胞).



Wigner-Seitz 原胞.

六棱柱.



2. 书上习题

1.3 证明体心立方之倒格子为面心立方, 反之亦然.

Pf: 由于倒格子之倒格子为正格子, 只证第一部分. (fcp ⇐ ccp)

$$\begin{cases} \vec{a_1} = \frac{a}{2}(\vec{i}+\vec{j}+\vec{k}) \\ \vec{a_2} = \frac{a}{2}(-\vec{i}+\vec{j}-\vec{k}) \\ \vec{a_3} = \frac{a}{2}(-\vec{i}-\vec{j}+\vec{k}) \end{cases} \qquad V = \frac{1}{2}a^3.$$

那么 $\vec{b}_1=\frac{2\pi}{V}(\vec{a}_2\times\vec{a}_3)=\frac{2\pi}{\frac{1}{2}a^3}\cdot(\frac{a}{2})^2\ (-\vec{i}+\vec{j}-\vec{k})\times(-\vec{i}-\vec{j}+\vec{k})$

$=\pi/a\ (\vec{k}+\vec{j}+\vec{k}+\vec{i}+\vec{j}-\vec{i})=\frac{2\pi}{a}(\vec{j}+\vec{k})$

$\vec{b}_2=2\pi/a\ (-\vec{k}+\vec{j}+\vec{k}-\vec{i}+\vec{j}-\vec{i})=2\pi/a\ (\vec{j}-\vec{i})$

$\vec{b}_3=\pi/a\ (\vec{k}+\vec{j}+\vec{k}-\vec{i}-\vec{j}-\vec{i})=2\pi/a\ (\vec{k}-\vec{i})$

为面心立方倒格矢. 证毕.

1.4 证明:

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

由于 $(\vec{A}\times\vec{B})\times\vec{C}=(\vec{A}\cdot\vec{C})\cdot\vec{B}-(\vec{A}\cdot\vec{B})\cdot\vec{C}$

因而 $V^*=(\frac{2\pi}{V_c})^3\left[(\vec{a}_2\times\vec{a}_3)\cdot\left(\left(-\vec{a}_1\cdot(\vec{a}_1\times\vec{a}_2)\right)\vec{a}_3+(\vec{a}_3\cdot(\vec{a}_1\times\vec{a}_2))\,\vec{a}_1\right)\right]$

$=(\frac{2\pi}{V_c})^3\cdot\left((\vec{a}_2\times\vec{a}_3)\cdot 0+V_c^2\right)$

$=(2\pi)^3/V_c$. 证毕.

1.5 $(h_1h_2h_3)$ 晶面族, 取最近邻原点晶面. 三截点为 $\vec{a}_1/h_1$, $\vec{a}_2/h_2$, $\vec{a}_3/h_3$.

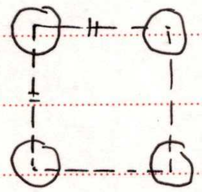
∴ 晶面上2个矢量 $\vec{a}_1/h_1-\vec{a}_2/h_2$, $\vec{a}_1/h_1-\vec{a}_3/h_3$.

由于 $(\vec{a}_i/h_i)\cdot\vec{G}_{h_1h_2h_3}=\frac{\vec{a}_i\cdot\vec{b}_i h_i}{h_i}=2\pi$.

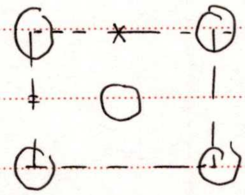
∴ 上两个矢量与 $\vec{G}_{h_1h_2h_3}$ 内积为0, 正交.

∴ $\vec{G}_{h_1h_2h_3}\perp(h_1h_2h_3)$. 证毕.

1.8 体心立方(100):



(110):



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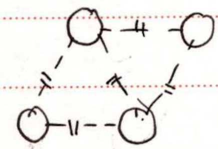
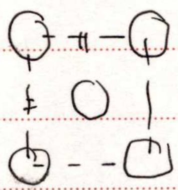


面心立方 (100)



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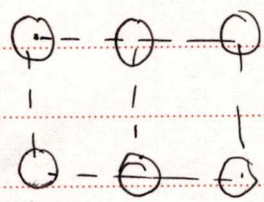

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